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Topological derivative method for an inverse problem modeled by the Schrödinger equation

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Abstract. This paper deals with an inverse potential problem whose forward problem is governed by Schrödinger equation. The inverse problem consists in the reconstruction of a set of anomalies embedded into a fluid from partial measurements of the substance concentration. Since the inverse problem, we are dealing with, is written in the form of an ill-posed boundary value problem, the idea is to rewrite it as a topology optimization problem. In particular, a shape functional is defined to measure the misfit of the solution obtained from the model and the data taken from the partial measurements. This shape functional is minimized with respect to a set of ball-shaped anomalies by using the concept of topological derivatives. It means that the shape functional is expanded asymptotically and then truncated up to the desired order term. The resulting expression is trivially minimized with respect to the parameters under consideration, leading to a non-iterative second order reconstruction algorithm. Finally, a numerical example is presented to show the effectiveness of the proposed reconstruction algorithm.

Keywords. Inverse problem, Schrödinger equation, topological derivatives, reconstruction method

1 Introduction

In this paper, we deal with an inverse potential problem in $\mathbb{R}^2$ whose corresponding forward problem is governed by the Schrödinger equation. The inverse problem under consideration is about the reconstruction of a set of anomalies embedded in a fluid with the help of partial measurements of the substance concentration. The inverse potential problem governed by the Schrödinger equation has been studied by many authors. See, for instance, [1, 3]. More precisely, let $\Omega \subset \mathbb{R}^2$ be an open and bounded domain with smooth boundary $\partial\Omega$. We consider a subset Ω_o of Ω where measurements of a scalar field of interest are taken. As illustrated in Figure 1(a), there may be an unknown number (denoted by $N^* \in \mathbb{Z}^+$) of isolated anomalies ω_i^* within the domain Ω, i.e., there is a set $\omega^* = \cup_{i=1}^{N^*}\omega_i^*$, with open connected components ω_i^* which satisfy $\overline{\omega_i^*} \cap \overline{\omega_j^*} = \emptyset$ for $i \neq j$ and $\overline{\omega_i^*} \cap \partial\Omega = \emptyset$, $\overline{\omega_i^*} \cap \Omega_o = \emptyset$ for each $i, j \in \{1, \cdots, N^*\}$.

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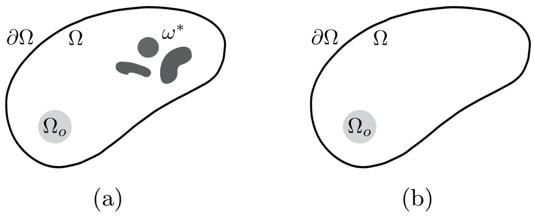

Figure 1: (a) Domain Ω with a set of anomalies ω^* and (b) Domain Ω without anomalies.

We consider the domain Ω as a bounded region representing a fluid medium which contains a different fluid substance within a subdomain ω^*. In this set up, the inverse problem consists in finding k_{ω^*} such that the substance concentration z satisfies the following boundary value problem

$$\left\{ \begin{array}{rcll} -\Delta z + k_{\omega^*} z & = & 0 & \text{in } \Omega, \\ z & = & g & \text{on } \partial\Omega, \end{array} \right. \tag{1}$$

where the given Dirichlet data g is smooth and the parameter k_{ω^*} is such that $k_{\omega^*} = 0$ in $\Omega \setminus \omega^*$ and $k_{\omega^*} = k$ in ω^*, with $k \in \mathbb{R}^+$. Now, for an initial guess k_ω of k_{ω^*}, we consider the substance concentration field u to be the solution to the boundary value problem

$$\left\{ \begin{array}{rcll} -\Delta u + k_{\omega} u & = & 0 & \text{in } \Omega, \\ u & = & g & \text{on } \partial\Omega, \end{array} \right. \tag{2}$$

where k_ω is such that $k_\omega = 0$ in $\Omega \setminus \omega$ and $k_\omega = k$ in ω.

The quantity k_{ω^*} is unknown and hence z but we assume that z can be measured in Ω_o. We would like to find k_{ω^*} with the help of measurements of z taken in Ω_o. If we want to look for the an appropriate k_{ω^*}, we wish u to agree with z in Ω_o i.e. we want $u = z_{|\Omega_o}$.

Since the inverse problem (1) does not have a unique solution when we want to determine both, the topology of ω^* and the value k, we assume that the material property of fluid anomalies k is known and we reconstruct the support of the anomalies ω^* with the help of the measurements of z taken in Ω_o. It is also well known that the inverse problem of finding ω^* in (1) for a given k still leads to an ill-posed boundary value problem. Therefore, the idea is to rewrite it as a topology optimization problem. For this purpose, we consider a weaker formulation of the inverse problem (1) which consists in solving the topology optimization problem

$$\underset{\omega \subset \Omega}{\text{Minimize}} \;\; \mathcal{J}_\omega \left(u^1, \cdots, u^M\right) = \sum_{m=1}^{M} \int_{\Omega_o} (u^m - z^m)^2 \,, \tag{3}$$

where $M \in \mathbb{Z}^+$ is the number of observations, z^m denotes the measurement of concentration of the fluid in Ω_o and u^m denotes the solution of the boundary value problem (2) corresponding to the Dirichlet data g^m for $m = 1, \cdots, M$. Notice that, the minimizer of the topology optimization problem (3) produces the best approximation to ω^*, solution of the inverse problem (1), in an appropriate sense.

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In particular, problem (3) is minimized with respect to a set of ball-shaped anomalies by using the concept of topological derivatives [5]. It means that the shape functional $\mathcal{J}_\omega\left(u^1,\cdots,u^M\right)$ is expanded asymptotically and then truncated up to the desired order term. The resulting expression is trivially minimized with respect to the parameters under consideration, leading to a non-iterative second order reconstruction algorithm.

The paper is organized as follows. In Section 2, the mathematical formulation of the inverse problem is described as a topology optimization problem taking into account the topological derivative concept. In Section 3, the asymptotic expansion of the shape functional is presented. Based on this asymptotic expansion, a non-iterative reconstruction algorithm is devised and a numerical example is presented in Section 4. Conclusions are discussed in Section 5.

2 Topology optimization setting

The inverse problem (1) has been written in the form of a topology optimization problem (3). It is well known that a quite general approach for dealing with such class of problems is based on the concept of topological derivative, which consists in expanding the shape functional $\mathcal{J}_\omega\left(u^1,\cdots,u^M\right)$ with respect to the parameters depend upon a set of small inclusions. Since the topological derivative does not depend on the initial guess of the unknown topology ω^*, we start with the unperturbed domain by setting $\omega=\emptyset$, see Figure 1(b). More precisely, we consider

$$\mathcal{J}_0\left(u_0^1,\cdots,u_0^M\right)=\sum_{m=1}^{M}\int_{\Omega_o}\left(u_0^m-z^m\right)^2, \tag{4}$$

where u_0^m be the solution of the unperturbed boundary value problem

$$\left\{\begin{array}{rcll} -\Delta u_0^m &=& 0 & \text{in } \Omega,\\ u_0^m &=& g^m & \text{on } \partial\Omega. \end{array}\right. \tag{5}$$

Here, we are considering the topology optimization problem (3) for the ball-shaped anomalies and hence we define the topologically perturbed counter-part of (5) by introducing $N\in\mathbb{Z}^+$ number of small circular inclusions $B_{\varepsilon_i}(x_i)$ with center at $x_i\in\Omega$ and radius ε_i for $i=1,\cdots,N$. The set of inclusions can be denoted as $B_\varepsilon(\xi)=\cup_{i=1}^N B_{\varepsilon_i}(x_i)$, where $\xi=(x_1,\ldots,x_N)$ and $\varepsilon=(\varepsilon_1,\ldots,\varepsilon_N)$. Moreover, we assume that $\overline{B_\varepsilon}\cap\partial\Omega=\emptyset$, $\overline{B_\varepsilon}\cap\Omega_o=\emptyset$ and $\overline{B_{\varepsilon_i}(x_i)}\cap\overline{B_{\varepsilon_j}(x_j)}=\emptyset$ for each $i\neq j$ and $i,j\in\{1,\cdots,N\}$. The shape functional associated with the topologically perturbed domain is written as

$$\mathcal{J}_\varepsilon\left(u_\varepsilon^1,\cdots,u_\varepsilon^M\right)=\sum_{m=1}^{M}\int_{\Omega_o}\left(u_\varepsilon^m-z^m\right)^2 \tag{6}$$

with u_ε^m be the solution of the perturbed boundary value problem

$$\left\{\begin{array}{rcll} -\Delta u_\varepsilon^m+k_\varepsilon u_\varepsilon^m &=& 0 & \text{in } \Omega,\\ u_\varepsilon^m &=& g^m & \text{on } \partial\Omega, \end{array}\right. \tag{7}$$

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where the parameter k_ε is such that $k_\varepsilon = 0$ in $\Omega \setminus B_\varepsilon(\xi)$ and $k_\varepsilon = k$ in $B_\varepsilon(\xi)$.

As mentioned earlier, the topological derivatives measure the sensitivity of the shape functional with respect to the parameters (ε, ξ) depending upon a set of small inclusions $B_\varepsilon(\xi)$. Therefore, our idea is to obtain the number, shape and locations of the inclusions that produce the best approximation to the anomaly ω^* by using the concept of topological derivatives. Proceeding in this way, we are interested in expanding the shape functional $\mathcal{J}_\varepsilon\left(u_\varepsilon^1, \ldots, u_\varepsilon^M\right)$ defined in (6) with respect to the volume (Lebesgue measure) of the two-dimensional ball $B_{\varepsilon_i}(x_i)$, i.e., $|B_{\varepsilon_i}(x_i)| = \pi\varepsilon_i^2 =: \alpha_i$. We start by simplifying the difference between the perturbed shape functional $\mathcal{J}_\varepsilon\left(u_\varepsilon^1, \cdots, u_\varepsilon^M\right)$ and its unperturbed counter-part $\mathcal{J}_0\left(u_0^1, \cdots, u_0^M\right)$ defined in (6) and (4), respectively, as follows

$$\mathcal{J}_\varepsilon(u_\varepsilon) - \mathcal{J}_0(u_0) = \sum_{m=1}^{M} \int_{\Omega_o} \left[2\left(u_\varepsilon^m - u_0^m\right)\left(u_0^m - z^m\right) + \left(u_\varepsilon^m - u_0^m\right)^2\right], \tag{8}$$

where $u_\varepsilon = \left(u_\varepsilon^1, \cdots, u_\varepsilon^M\right)$ and $u_0 = \left(u_0^1, \cdots, u_0^M\right)$.

For $m = 1, \cdots, M$, let us consider the following ansätz for the expansion of u_ε^m with respect to α_i (observe that α_i depends on ε_i):

$$u_\varepsilon^m(x) = u_0^m(x) + k\sum_{i=1}^{N} \alpha_i h_i^{\varepsilon,m}(x) + k^2 \sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i\alpha_j h_{ij}^{\varepsilon,m}(x) + \tilde{u}_\varepsilon^m(x), \tag{9}$$

where, for each $i = 1, \cdots, N$ and $m = 1, \cdots, M$, $h_i^{\varepsilon,m}$ is the solution of

$$\left\{\begin{array}{rcll} \Delta h_i^{\varepsilon,m} & = & \dfrac{u_0^m}{|B_{\varepsilon_i}(x_i)|}\chi_{B_{\varepsilon_i}(x_i)} & \text{in } \Omega, \\ h_i^{\varepsilon,m} & = & 0 & \text{on } \partial\Omega. \end{array}\right. \tag{10}$$

We write $h_i^{\varepsilon,m}$ as a sum of three functions p_i^ε, q_i and $\tilde{h}_i^{\varepsilon,m}$. In other words, $h_i^{\varepsilon,m} = u_0^m(x_i)(p_i^\varepsilon + q_i) + \tilde{h}_i^{\varepsilon,m}$, where p_i^ε is a particular solution obtained by the convolution of $|B_{\varepsilon_i}(x_i)|^{-1}\chi_{B_{\varepsilon_i}(x_i)}$ with the kernel of the Laplacian. More precisely,

$$p_i^\varepsilon(x) = \frac{1}{|B_{\varepsilon_i}(x_i)|}\int_{B_{\varepsilon_i}(x_i)} \frac{1}{2\pi}\log\|y - x\| dy. \tag{11}$$

Outside the ball $B_{\varepsilon_i}(x_i)$, we can simplify (11) to obtain

$$p_i(x) := p_i^\varepsilon(x) = \frac{1}{2\pi}\log\|x_i - x\| \quad \forall x \in \Omega \setminus \overline{B_{\varepsilon_i}(x_i)}. \tag{12}$$

Observe that $p_i(x)$ does not depend on ε_i. Additionally, q_i is the solution to the homogeneous boundary value problem

$$\left\{\begin{array}{rcll} \Delta q_i & = & 0 & \text{in } \Omega, \\ q_i & = & -\dfrac{1}{2\pi}\log\|x_i - x\| & \text{on } \partial\Omega \end{array}\right. \tag{13}$$

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and $\tilde{h}_i^{\varepsilon,m}$ solves the boundary value problem

$$\left\{\begin{array}{rcll} \Delta\tilde{h}_i^{\varepsilon,m} & = & \dfrac{u_0^m - u_0^m(x_i)}{|B_{\varepsilon_i}(x_i)|}\chi_{B_{\varepsilon_i}(x_i)} & \text{in } \Omega, \\ \tilde{h}_i^{\varepsilon,m} & = & 0 & \text{on } \partial\Omega. \end{array}\right. \tag{14}$$

Taking into account the decomposition of $h_i^{\varepsilon,m}$ given by $h_i^{\varepsilon,m} = u_0^m(x_i)(p_i^\varepsilon + q_i) + \tilde{h}_i^{\varepsilon,m}$, we can introduce the notations $h_i := p_i + q_i$ and $h_i^\varepsilon := p_i^\varepsilon + q_i$ with p_i^ε, p_i as given in (11), (12), respectively. In (9), $h_{ij}^{\varepsilon,m}$ and $\tilde{u}_\varepsilon^m$ are the solutions of the following boundary value problems

$$\left\{\begin{array}{rcll} \Delta h_{ij}^{\varepsilon,m} & = & \dfrac{h_j^{\varepsilon,m}}{|B_{\varepsilon_i}(x_i)|}\chi_{B_{\varepsilon_i}(x_i)} & \text{in } \Omega, \\ h_{ij}^{\varepsilon,m} & = & 0 & \text{on } \partial\Omega, \end{array}\right. \tag{15}$$

and

$$\left\{\begin{array}{rcll} -\Delta\tilde{u}_\varepsilon^m + k_\varepsilon\tilde{u}_\varepsilon^m & = & -\Phi_\varepsilon^m & \text{in } \Omega, \\ \tilde{u}_\varepsilon^m & = & 0 & \text{on } \partial\Omega, \end{array}\right. \tag{16}$$

respectively. In problem (16), we have $\Phi_\varepsilon^m = k^3\sum_{i,j,l=1}^N |B_{\varepsilon_j}(x_j)||B_{\varepsilon_l}(x_l)|h_{jl}^{\varepsilon,m}\chi_{B_{\varepsilon_i}(x_i)}$.

In order to simplify further calculations, let us introduce an adjoint state v^m as the solution of the following auxiliary boundary value problem

$$\left\{\begin{array}{rcll} -\Delta v^m & = & (u_0^m - z^m)\,\chi_{\Omega_o} & \text{in } \Omega, \\ v^m & = & 0 & \text{on } \partial\Omega. \end{array}\right. \tag{17}$$

3 Topological asymptotic expansion

Now, we have all elements to evaluate the difference (8) explicitly. In fact, the topological asymptotic expansion of the shape functional $\mathcal{J}_\varepsilon(u_\varepsilon)$ can be written as

$$\mathcal{J}_\varepsilon(u_\varepsilon) = \mathcal{J}_0(u_0) - \alpha\cdot d(\xi) + G(\xi)\alpha\cdot\operatorname{diag}(\alpha\otimes\log\alpha) + \frac{1}{2}H(\xi)\alpha\cdot\alpha + o(|\alpha|^2), \tag{18}$$

where $\alpha = (\alpha_1, \cdots, \alpha_N)$. In addition, the vector $d\in\mathbb{R}^N$, the matrix $G\in\mathbb{R}^N\times\mathbb{R}^N$ and the Hessian matrix $H\in\mathbb{R}^N\times\mathbb{R}^N$ in the above expression are defined as

$$d_i := 2k\sum_{m=1}^M u_0^m(x_i)v^m(x_i), \tag{19}$$

$$G_{ii} := -\frac{k^2}{2\pi}\sum_{m=1}^M u_0^m(x_i)v^m(x_i), \quad G_{ij} = 0, \quad \text{if} \quad i\neq j \tag{20}$$

and

$$\begin{aligned} H_{ii} := \frac{1+\log\pi^2}{2\pi}k^2\sum_{m=1}^M u_0^m(x_i)v^m(x_i) - 4k^2\sum_{m=1}^M u_0^m(x_i)v^m(x_i)q_i(x_i) \\ -\frac{k}{\pi}\sum_{m=1}^M \nabla u_0^m(x_i)\cdot\nabla v^m(x_i) + 2k^2\sum_{m=1}^M (u_0^m(x_i))^2\int_{\Omega_o} h_i^2, \end{aligned} \tag{21}$$

$$H_{ij} := -2k^2 \sum_{m=1}^{M} [u_0^m(x_j)h_j(x_i)v^m(x_i) + u_0^m(x_i)h_i(x_j)v^m(x_j)] + 2k^2 \sum_{m=1}^{M} u_0^m(x_i)u_0^m(x_j) \int_{\Omega_o} h_i h_j, \quad \text{if} \quad i \neq j, \quad (22)$$

respectively, for $i, j = 1, \cdots, N$. The vector $d(\xi)$ and the Hessian matrix $H(\xi)$ are called the first and second order topological derivative of the shape functional $\mathcal{J}_\varepsilon(u_\varepsilon)$, respectively.

4 Numerical results

The expression on the right-hand side of (18) depends on the number of anomalies N, their sizes α and locations ξ. Thus, from (18), we can define $\delta J(\alpha, \xi, N) := -\alpha \cdot d(\xi) + G(\xi)\alpha \cdot \text{diag}(\alpha \otimes \log \alpha) + \frac{1}{2}H(\xi)\alpha \cdot \alpha$. The derivative of the function $\delta J(\alpha, \xi, N)$ with respect to the variable α yields the first order optimality condition, namely, $\langle D_\alpha \delta J, \beta \rangle = [(H(\xi) + G(\xi))\,\alpha + 2G(\xi)\text{diag}(\alpha \otimes \log \alpha) - d(\xi)] \cdot \beta = 0, \forall \beta$, which leads to the non-linear system of the form

$$(H(\xi) + G(\xi))\,\alpha + 2G(\xi)\text{diag}(\alpha \otimes \log \alpha) = d(\xi) \quad (23)$$

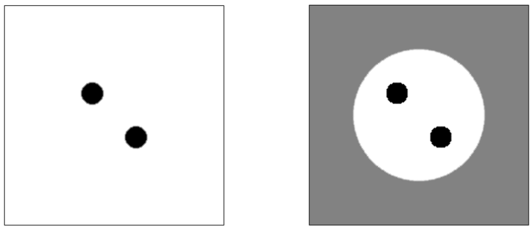
with the entries of the vector $d \in \mathbb{R}^N$ and the matrices $G,\ H \in \mathbb{R}^N \times \mathbb{R}^N$ defined in (19), (20), (21) and (22), respectively.

The quantity α solution of (23) becomes a function of the locations ξ, namely $\alpha = \alpha(\xi)$, and its value is obtained by using the Newton's method. Let us now replace the solution of (23) into the expression for $\delta J(\alpha, \xi, N)$. Therefore, the optimal locations $\xi^\star$ can be trivially obtained from a combinatorial search over the domain Ω, solution to the following minimization problem $\xi^\star = \text{argmin}_{\xi \in X} \left\{\delta J(\alpha(\xi), \xi, N) = -\frac{1}{2}\left(d(\xi) + G(\xi)\alpha(\xi)\right) \cdot \alpha(\xi)\right\}$, where X is the set of admissible anomalies locations. Finally, the optimal sizes are given by $\alpha^\star = \alpha(\xi^\star)$. In summary, our method is able to find in one step the optimal sizes $\alpha^\star$ and theirs locations $\xi^\star$ for a given N. The above procedure written in pseudo-code format can be found in [2, 4].

Now, we present a numerical example in order to demonstrate the effectiveness of the method proposed in the earlier sections of this paper. We consider the geometric domain $\Omega = (-0.5, 0.5) \times (-0.5, 0.5)$ which is discretized using three-node finite element scheme. Considering the mesh and the subdomain Ω_o, we form a uniform subgrid with a set of feasible nodes X within which a combinatorial search is performed in order to find the optimal size $\alpha^\star$ and the appropriate center $\xi^\star$ of the embedded anomalies. In the Figure 2, we represent anomalies by black, the subdomain Ω_o by gray and the remaining domain $\Omega \setminus \Omega_o$ by white colors.

The example: Two circular regions with centers located at $x_1^* = (-0.1, 0.1)$, $x_2^* = (0.1, -0.1)$ and with radius $\varepsilon_1^* = \varepsilon_2^* = 0.05$ are considered as the target anomalies. The concentration of the fluid is measured in $\Omega_o = \Omega \setminus B_\rho(0,0)$ with $B_\rho(0,0) = \{x \in \mathbb{R}^2 : \|x\| < \rho\}$, where $\rho = 0.3$. In the current setting, we take only one observation by taking into account the Dirichlet data $g = 1$. The domain Ω containing the two target anomalies

ω_1^* and ω_2^* is illustrated in Figure 2(a). We reconstruct the anomalies by considering $k = 1$. The combinatorial search was conducted on the subgrid of 57 nodes within $\Omega \setminus \Omega_o$. We successfully find the exact location of the centers x_1^* and x_2^* of the anomalies ω_1^* and ω_2^*, respectively. The radius obtained were $\varepsilon_1^\star = \varepsilon_2^\star = 0.04943$ which are approximately equal to the true value. We demonstrate the numerical result in Figure 2(b).



(a) (b)

Figure 2: (a) Target domain and (b) the respective result.

5 Conclusions

In this paper a non-iterative reconstruct method for an inverse potential problem modeled by the Schrödinger equation is proposed. The method is based on the topological derivatives of shape functionals associated with the inverse problems. One the one hand, the algorithm devised is able to reconstruct the embedded anomalies in one step and it is independent of any initial guess. One the other hand, an accurate reconstruction can requires more than one observation depending on the setting of the subdomain where the measurements of concentration of the fluid are taken and the number of embedded anomalies.

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