Application of the Hybrid Stochastic- Deterministic Minimization Method to a Surface Data Inverse Scattering Problem

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Abstract. A method for the identification of small inhomogeneities from a surface data is presented in the framework of an inverse scattering problem for the Helmholtz equation. Using the assumptions of smallness of the scatterers one reduces this inverse problem to an identification of the positions of the small scatterers. These positions are found by a global minimization search. Such a search is implemented by a novel Hybrid Stochastic-Deterministic Minimization method. The method combines random tries and a deterministic minimization. The effectiveness of this approach is illustrated by numerical experiments. In the modeling part our method is valid when the Born approximation fails. In the numerical part, an algorithm for the estimate of the number of the small scatterers is proposed.

1 Introduction

In many applications it is essential to find small inhomogeneities from surface data. For example, such a problem arises in ultrasound mammography, where small inhomogeneities are cancer cells. Current X-ray mammography will be replaced by the ultrasound one because X-ray mammography has a high probability of creating new cancer cells in a woman’s breast in the course of taking the mammography test. Other examples include the problem of finding small holes and cracks in metals and other materials, or the mine detection. The scattering theory for small scatterers originated in the classical works of Lord Rayleigh. It was developed in [15] and [16], where analytical formulas for the scattering matrix were derived for the acoustic and

1991 Mathematics Subject Classification. Primary 35R30, 65K10; Secondary 86A22.
electromagnetic scattering problems. In [13] and [17] inverse scattering problems for small bodies are considered. In [18] the problem of identification of small subsurface inhomogeneities from surface data was posed and its possible applications were discussed. In [11] the results of the numerical experiments are presented for the problem of finding one small inhomogeneity from surface data. In [7] a method for finding small inhomogeneities from tomographic data is proposed. The main result of our paper is the new optimization procedure which can be used for actual finding the small subsurface inhomogeneities from surface scattering data. Our numerical results demonstrate that the method proposed in this paper is potentially of practical importance.

Consider a point source $y$ of monochromatic acoustic waves on the surface of the earth. Let $u(x, y, k)$ be acoustic pressure at the point $x$, and $k > 0$ be the wavenumber. The governing equation is:

$$\nabla^2 u + k^2 v(x) u = -\delta(x - y) \quad \text{in} \quad R^3, \quad (1.1)$$

$u$ satisfies the radiation condition at infinity, and $v(x)$ is the inhomogeneity in the velocity profile, $x = (x_1, x_2, x_3)$.

Let us assume that $v(x)$ is a bounded function vanishing outside of the domain $D = \bigcup_{m=1}^{M} D_m$ which is the union of $M$ small nonintersecting domains $D_m$, all of them are located in the lower half-space $R^3_- = \{x : x_3 < 0\}$. Smallness is understood in the sense $k \rho \ll 1$, where $\rho := \frac{1}{J} \max_{1 \leq m \leq M} \{\text{diam } D_m\}$, and diam $D$ is the diameter of the domain $D$. Practically $k \rho \ll 1$ means that $k \rho < 0.1$, in some cases $k \rho < 0.2$ is sufficient for obtaining acceptable numerical results. The background velocity in (1.1) equals to 1, but we can consider the case of fairly general background velocity [17].

Denote $\tilde{z}_m$ and $\tilde{v}_m$ the positions of the gravity center of $D_m$ and the total intensity of the $m$-th inhomogeneity $\tilde{v}_m := \int_{D_m} v(x) dx$. Assume that $\tilde{v}_m \neq 0$.

The inverse problem to be solved is:

**IP**: Given $u(x, y, k)$ for all $(x, y)$ on $P := \{x : x_3 = 0\}$ at a fixed $k > 0$, find the number $M$ of small inhomogeneities, the positions $\tilde{z}_m$ of the inhomogeneities, and their intensities $\tilde{v}_m$.

2 Method of solution

Let us introduce the following notations:

$$P := \{x : x_3 = 0\}, \quad (2.1)$$

$$\{x_j, y_j\} := \xi_j, \quad 1 \leq j \leq J, \quad x_j, y_j \in P, \quad (2.2)$$

are the points at which the data $u(x_j, y_j, k)$ are collected,

$$k > 0 \quad \text{is fixed}, \quad (2.3)$$

$$g(x, y, k) := \frac{\exp(ik|x - y|)}{4\pi|x - y|}, \quad (2.4)$$

$$G_j(z) := G(\xi_j, z) := g(x_j, z, k)g(y_j, z, k), \quad (2.5)$$
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\[ f_j := \frac{u(x_j, y_j, k) - g(x_j, y_j, k)}{k^2}, \quad (2.6) \]

\[ \Phi(z_1, \ldots, z_M, v_1, \ldots, v_M) := \sum_{j=1}^{J} \left| f_j - \sum_{m=1}^{M} G_j(z_m)v_m \right|^2. \quad (2.7) \]

The proposed method for solving the (IP) consists in finding the global minimizer of function (2.7). This minimizer \( (\tilde{z}_1, \ldots, \tilde{z}_M, \tilde{v}_1, \ldots, \tilde{v}_M) \) gives the estimates of the positions \( \tilde{z}_m \) of the small inhomogeneities and their intensities \( v_m \).

The above approach can be justified as follows. The Helmholtz equation (1.1) with the radiation condition is equivalent to the integral equation

\[ u(x, y, k) = g(x, y, k) + k^2 \sum_{m=1}^{M} \int_{D_m} g(x, z, k)v(z)u(z, y, k)dz. \quad (2.8) \]

For small inhomogeneities the integral on the right-hand side of (2.8) can be approximately written as

\[ \int_{D_m} g(x, z, k)v(z)u(z, y, k)dz \approx \int_{D_m} g(x, z, k)v(z)g(z, y, k)dz \]

\[ \approx G(x, y, \xi_m) \int_{D_m} v(z)dz := G(\xi, \xi_m)v_m, \quad 1 \leq m \leq M, \quad (2.9) \]

where \( \xi_m \) is a point close to \( \tilde{z}_m \), and \( u(z, y, k) \) under the sign of the integral in (2.8) can be replaced by \( g(x, y, k) \) with a small error \( \varepsilon^2 \) provided that

\[ \varepsilon := c_0 M(k\rho)^2 \ll 1, \quad (2.10) \]

where

\[ \rho = \max_{1 \leq m \leq M} \rho_m, \quad \rho_m := \frac{1}{2} \text{diam} D_m, \quad c_0 := \max_{x \in \mathbb{R}^3} |v(x)|, \quad (2.11) \]

and \( M \) is the number of inhomogeneities.

Note that the sufficient condition for the validity of the Born approximation for equation (2.8), is the smallness of the norm in \( L^2(D) \) of the integral operator in (2.8). The above condition can be written as

\[ Mc_0 k^2 \rho^2 \ll 1. \quad (*) \]

If \( x, y \in P \), then

\[ |u - g| < O(Mk^2c_0\rho^3d^{-2}), \]

where \( d > 0 \) is the minimal distance from \( D_m \) to \( P \).

The relative error of the first approximation in (2.9) for \( x, y \in P \) is \( O(Mk^2c_0\rho^3d^{-1}) \), where \( d > 0 \) is the minimal distance from \( D_m \) to \( P \). If \( d > 0 \) is not too small, \( c_0\rho^3 := V \) is not too large, then the above error is small if

\[ \epsilon_1 := M^2c_0\rho^3d^{-1} << 1, \quad (**) \]

where \( \epsilon_1 \) is a dimensionless quantity. Condition (*) can be written as \( \frac{Mk^2V}{\rho} \ll 1 \). This condition is much stronger than condition (**), which can be written as \( \frac{k^2V}{\rho} \ll 1 \), since \( d \gg \rho \). Therefore the approximation (2.9) is applicable when the Born approximation may fail.

If the condition

\[ c_0\rho^3 = \text{const} \quad \text{as} \quad \rho \to 0 \quad (***) \]
holds, then condition (\(^*\)) for the validity of the Born approximation is violated because \(\frac{d^2\xi_j}{d\rho^2} \to \infty\) as \(\rho \to 0\).

Condition (\(***\)) corresponds to the scattering by delta-type inhomogeneities. For such scattering the Born approximation is not applicable, but a modified representation of the type (2.9) is valid (see \[1\], p.113, formula (1.1.33), and \[8\], \[19\]).

From (2.9) and (2.6) it follows that

\[ f_j \approx \sum_{m=1}^{M} G_j(z_m) v_m, \quad G_j(z_m) := G(\xi_j, z_m, k) \] (2.12)

Therefore, parameters \(\tilde{z}_m\) and \(\tilde{v}_m\) can be estimated by the least-squares method if one finds the global minimum of the function (2.7):

\[ \Phi(z_1, \ldots, z_M, v_1, \ldots, v_M) = \min \] (2.13)

The function \(\Phi\) depends on \(M\) unknown points \(z_m \in \mathbb{R}^3\), and \(M\) unknown parameters \(v_m, \quad 1 \leq m \leq M\). The parameter \(M\), the number of the small inhomogeneities, is estimated by the algorithm described in Sec. 3 below, see also a discussion in the beginning of Section 4.

### 3 Hybrid Stochastic-Deterministic Method

Let the inhomogeneities be located within a box

\[ B = \{ (x_1, x_2, x_3) : -a < x_1 < a, \ -b < x_2 < b, \ 0 < x_3 < c \} \] (3.1)

and their intensities satisfy

\[ 0 \leq v_m \leq v_{\text{max}} \] (3.2)

Then, given the location of the points \(z_1, z_2, \ldots, z_M\), the minimum of \(\Phi\) in (2.13) with respect to the intensities \(v_1, v_2, \ldots, v_M\) can be found by minimizing the quadratic function in (2.7) over the region satisfying (3.2). This can be done using normal equations for (2.7) and projecting the resulting point back onto the region defined by (3.2). Denote the result of this minimization by \(\tilde{\Phi}\), that is

\[ \tilde{\Phi}(z_1, z_2, \ldots, z_M) = \min \{ \Phi(z_1, z_2, \ldots, z_M, v_1, v_2, \ldots, v_M) : 0 \leq v_m \leq v_{\text{max}}, \quad 1 \leq m \leq M \} \] (3.3)

Now the minimization problem (2.13) is reduced to the 3M-dimensional restrained minimization

\[ \tilde{\Phi}(z_1, z_2, \ldots, z_M) = \min \quad z_m \in B, \quad 1 \leq m \leq M. \] (3.4)

Note, that the dependency of \(\tilde{\Phi}\) on its 3M variables (the coordinates of the points \(z_m\)) is highly nonlinear. In particular, this dependency is complicated by the computation of the minimum in (3.3) and the consequent projection onto the admissible set \(B\). Thus, an analytical computation of the gradient of \(\tilde{\Phi}\) is not computationally efficient. We have used Powell’s quadratic minimization method to find local minima. This method uses a special procedure to numerically approximate the gradient, and it can be shown to exhibit the same type of quadratic convergence as conjugate gradient type methods (see \[4\]).

In addition, the exact number of the original inhomogeneities \(M_{\text{orig}}\) is unknown, and its estimate is a part of the inverse problem. In the HSD algorithm described
below this task is accomplished by taking an initial number $M$ sufficiently large, so that

$$M_{\text{orig}} \leq M,$$  \hspace{1cm} (3.5)

which, presumably, can be estimated from physical considerations. After all, our goal, is to find only the strongest inclusions, since the weak ones cannot be distinguished from the background noise. The Reduction Procedure (see below) allows the algorithm to seek the minimum of $\Phi$ in a lower dimensional subsets of the admissible set $B$, thus finding the estimated number of inclusions $M$. Still another difficulty in the minimization is a large number of local minima of $\Phi$. While this phenomena is well known for the objective functions arising in various inverse problems, we illustrate this point on Figure 1.

The original configuration $(\tilde{z}_1, \tilde{z}_2, \ldots, \tilde{z}_M, \tilde{v}_1, \tilde{v}_2, \ldots, \tilde{v}_M), M_{\text{orig}} = 6$ is presented in Table 1. Figure 1 shows the values of the function $\Phi(z_r, z_2, \tilde{z}_4, \tilde{z}_5, \tilde{z}_6)$, where

$$z_r = (r, 0, 0.520), \quad -2 \leq r \leq 2$$
and
\[ z_2 = (-1, 0.3, 0.580) . \]

The plot shows multiple local minima and almost flat regions.

A direct application of a gradient type method to such a function would result in finding a local minimum, which may or may not be the sought global one. In the example above, such a method would usually be trapped in a local minimum located at \( r = -2, r = -1.4, r = -0.6, r = 0.2 \) or \( r = 0.9 \). While the desired global minimum at \( r = 1.6 \) will be found only for a sufficiently close initial guess \( 1.4 < r < 1.9 \). While various global minimization methods are known (see below), we found that the most efficient way to accomplish the task for this Inverse Problem was to design a new method (HSD) combining both the stochastic and the deterministic approach to the global minimization. Deterministic minimization algorithms with or without the gradient computation, such as the conjugate gradient methods, are known to be highly efficient (see [4, 6, 16]). However, the initial guess should be chosen sufficiently close to the sought minimum. Also such algorithms, as we mentioned above, tend to be trapped at a local minimum, which is not necessarily close to a global one. A new deterministic method is proposed in [2], and [8], which is quite efficient according to [8]. On the other hand, various stochastic minimization algorithms, e.g. the simulated annealing method [12, 13], are more likely to find a global minimum, but their convergence can be very slow. We have tried a variety of minimization algorithms to find an acceptable minimum of (3.4) or (2.13). Among them were the Levenberg-Marquardt Method, Conjugate Gradients, Downhill Simplex, and Simulated Annealing Method. None of them produced consistent satisfactory results.

Among the minimization methods combining random and deterministic searches we mention Deep’s method [5] and a variety of clustering methods [20], [21]. An application of these methods to the particle identification using light scattering is described in [22]. The clustering methods are quite robust but, usually, require a significant computational effort. The HSD method is a combination of a reduced sample random search method with certain ideas from Genetic Algorithms (see e.g. [9]). It is very efficient and seems especially well suited for low dimensional global minimization. Further research is envisioned to study its properties in more detail, and its applicability to other problems.

While the steps of the Hybrid Stochastic-Deterministic (HSD) method are outlined below, its basic idea is to start with a random search for the minimum. If at a certain configuration \( x_s \) the minimized function is judged to be sufficiently small, this configuration is a candidate for the initial guess of a deterministic minimization method. However, this minimization is applied only after the points with smaller intensities in \( x_s \) are dropped (Step 2 below), and all sufficiently close points are eliminated (Step 3). Now a deterministic minimization is performed in the resulting lower dimensional subspace. The minimizer \( x_d \) is likely to represent at least some of the sought inhomogeneities. These points are supplemented with randomly chosen ones to obtain a full configuration (Step 1). In this manner the iterations of the random searches and the deterministic minimization continue till a tolerance criterion is satisfied. As the algorithm finds configurations with smaller and smaller values of the objective function, the likelihood of the finding the global minimum increases, while the irrelevant local minima are eliminated.

Let us outline the steps of a possible implementation of the HSD algorithm for the surface data inverse scattering problem described in Sections 1 and 2. We
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assume that all the inhomogeneities are located in a (known) box $B$, and $M$ is chosen according to (3.5). Our goal is to locate the points $\tilde{z}_1, \ldots, \tilde{z}_N$, $N \leq M$ which minimize $\tilde{\Phi}$ in (3.4).

Hybrid Stochastic-Deterministic (HSD) Method. Let $P_0, \epsilon_s, \epsilon_i, \epsilon_d, \epsilon$ be positive numbers. Let $N = 0$.

1. Generate randomly $M - N$ additional points $z_{N+1}, \ldots, z_M$ to obtain a full configuration $z_1, \ldots, z_M$. Compute $P_s = \tilde{\Phi}(z_1, z_2, \ldots, z_M)$. Save the resulting best fit intensities $v_m$, $1 \leq m \leq M$ (see 3.3). If $P_s < P_0 \epsilon_s$ then go to step 2, otherwise repeat this step 1.

2. Discharge all the points with the intensities $v_m$ satisfying $v_m < v_{max} \epsilon_i$. Now only $N \leq M$ points $z_1, z_2, \ldots, z_N$ remain in the box $B$.

3. If any two points $z_m, z_n$ in the above configuration satisfy $|z_m - z_n| < \epsilon_d D$, where $D = \text{diam}(B)$, then eliminate point $z_n$, change the intensity of point $z_m$ to $v_m + v_n$, and assign $N := N - 1$. This step is repeated until no further reduction in $N$ is possible.

4. Run a restrained deterministic minimization of $\tilde{\Phi}$ in $3N$ variables, with the initial guess at the configuration determined in step 3. Let the minimizer be $\tilde{z}_1, \ldots, \tilde{z}_N$. If $P = \tilde{\Phi}(\tilde{z}_1, \ldots, \tilde{z}_N) < \epsilon$ then save this configuration, and go to step 6, otherwise let $P_0 = P$, and proceed to the next step 5.

5. Keep intact $N$ points $\tilde{z}_1, \ldots, \tilde{z}_N$. If the number of random configurations has exceeded $T_{max}$ (the maximum number of random tries), then save the configuration and go to step 6, else go to step 1, and use these $N$ points there.

6. Repeat steps 1 through 5 $n_{max}$ times.

7. Find the configuration among the above $n_{max}$ ones, which gives the smallest value to $\tilde{\Phi}$. This is the best fit.

Step 1 is the stochastic part of the algorithm. In step 2 the points with low intensities are discharged, since they, most likely, are artifacts contributing on the level comparable with the background noise. Step 3 is the Reduction Procedure replacing two nearby inclusions with one of the joint intensity. Steps 2 and 3 lower the dimensionality of the minimization domain, thus greatly reducing the computational time needed to perform the deterministic minimization of the step 4. We have used Powell’s minimization method (see [4] for a detailed description) for the deterministic part, since this method does not need gradient computations and converges quadratically near quadratically shaped minima. Also, in step 1, an idea from the Genetic Algorithm’s approach [9] is implemented by keeping only the strongest representatives of the population and allowing a mutation for the rest.

4 Numerical results

The algorithm was tested on a variety of configurations. Here we present the results of just two typical numerical experiments illustrating the performance of the method. The data was simulated according to (2.12). In both experiments the box $B$ is taken to be

$$B = \{(x_1, x_2, x_3) : -a < x_1 < a, -b < x_2 < b, 0 < x_3 < c\},$$

with $a = 2$, $b = 1$, $c = 1$. The frequency $k = 5$, and the effective intensities $v_m$ are in the range from 0 to 2, (see Section 1). The values of the parameters defined in
Table 1 Actual inclusions.

| Inclusions | $x_1$ | $x_2$ | $x_3$ | $v$ |
|------------|-------|-------|-------|-----|
| 1          | 1.640 | -0.510| 0.520 | 1.200|
| 2          | -1.430| -0.500| 0.580 | 0.500|
| 3          | 1.220 | 0.570 | 0.370 | 0.700|
| 4          | 1.410 | 0.230 | 0.740 | 0.610|
| 5          | -0.220| 0.470 | 0.270 | 0.700|
| 6          | -1.410| 0.230 | 0.174 | 0.600|

Section 3 were chosen as follows

$$P_0 = 1, T_{max} = 1000, \epsilon_s = 0.5, \epsilon_i = 0.25, \epsilon_d = 0.1, \epsilon = 10^{-5}, n_{max} = 6$$

In both cases we searched for the same 6 inhomogeneities with the coordinates $x_1, x_2, x_3$ and the intensities $v$ shown in Table 1.

Parameter $M$ was set to 16, thus the only information on the number of inhomogeneities given to the algorithm was that their number does not exceed 16. This number was chosen to keep the computational time within reasonable limits. Still another consideration for the number $M$ is the aim of the algorithm to find the presence of the most influential inclusions, rather then all inclusions, which is usually impossible in the presence of noise and with the limited amount of data.

**Experiment 1.** In this case we used 12 sources and 21 detectors, all on the surface $x_3 = 0$. The sources were positioned at \{(-2 + 0.333 + 0.667i, -0.5 + 1.0j, 0), i = 0, \ldots, 5, j = 0, 1\}, that is 6 each along two lines $x_2 = -0.5$ and $x_2 = 0.5$. The detectors were positioned at \{(-2 + 0.667i, -1.0 + 1.0j, 0), i = 0, \ldots, 6, j = 0, 1, 2\}, that is seven detectors along each of the three lines $x_2 = -1, x_2 = 0$ and $x_2 = 1$. This corresponds to a mammography search, where the detectors and the sources are placed above the search area. The results of the identification are shown in Tables 2 and 3 for different noise levels $\delta$ in the data. See Figure 2. Table 3 has only 4 lines showing that the program has identified the presence of only 4 indicated inclusions, while missing the other 2.

To evaluate the performance of the algorithm, we have made 10 independent runs of the program for each of the noise levels $\delta = 0.00, \delta = 0.02, \text{and} \delta = 0.05$. In the noiseless case all 6 original inhomogeneities were identified every time. The program performed 2 or 3 deterministic minimizations in each run, spending from 30 to 80 percent of time in this minimization. For $\delta = 0.02$ the perfect identification also was obtained in every run. The deterministic minimization was performed 2-4 times, spending there 10 to 25% of the computational time. For $\delta = 0.05$ out of 10 runs the program found 4 and 5 inhomogeneities in one run each, and all 6 inhomogeneities in the rest 8 runs. The deterministic minimization was performed from 1 to 3 times in each run for the total of 5 to 20% of the computational time.

**Experiment 2.** In this case we used 8 sources and 22 detectors, all on the surface $x_3 = 0$. The sources were positioned at \{(-1.75 + 0.5i, 1.5j, 0), i = 0, \ldots, 7, j = 0, 1\}, that is all 8 along the line $x_2 = 1.5$. The detectors were positioned at \{(-2 + 0.4i, 1.0 + 1.0j, 0), i = 0, \ldots, 10, j = 0, 1\}, that is eleven detectors along each of the two lines $x_2 = 1$ and $x_2 = 2$. This corresponds to a mine search, where the detectors and the sources must be placed outside of the searched ground. The results of the identification are shown in Tables 4 and 5 for different noise levels $\delta$ in the data. See Figure 3. Because the sources and the detectors are further away from the inhomogeneities than in Experiment 1, this presents a
more difficult identification problem. The program identified less than 6 original inhomogeneities in some runs, thus Tables 4 and 5 contain less than 6 lines. As it can be seen, only the strongest inhomogeneities have been identified in these cases.

As in Experiment 1, we have made 10 independent runs of the program for each of the noise levels $\delta = 0.00$, $\delta = 0.02$, and $\delta = 0.05$. In the noiseless case $\delta = 0.00$, 5 or 6 original inhomogeneities were identified every time. In 3 runs an additional inhomogeneity (an artifact) has appeared. For $\delta = 0.02$ and $\delta = 0.05$ the identification has deteriorated, with 4 inhomogeneities recovered. The number of deterministic minimizations and the computational times spent doing them are somewhat higher than the ones reported for Experiment 1.

In general, the execution times were less than 2 minutes on a 333MHz PC. As it can be seen from the results, the method achieves a perfect identification in the Experiment #1 when no noise is present. The identification deteriorates in the presence of noise, as well as if the sources and detectors are not located directly above the search area. Still the inclusions with the highest intensity and the closest
ones to the surface are identified, while the deepest and the weakest are lost. This can be expected, since their influence on the cost functional is becoming comparable with the background noise in the data.

In summary, the proposed method for the identification of small inclusions can be used in geophysics, medicine and technology. It can be useful in the development of new approaches to ultrasound mammography. It can also be used for localization of holes and cracks in metals and other materials, as well as for finding mines from surface measurements of acoustic pressure and possibly in other problems of interest in various applications.

The HSD minimization method is a specially designed low-dimensional minimization method, which is well suited for many inverse type problems. The problems do not necessarily have to be within the Born approximation range. It is highly desirable to study applications of this method, and to compare its performance to other competitive methods.

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Figure 3 Inclusions and Identified objects for Experiment 2, $\delta = 0.00$. $x_3$ coordinate is not shown.

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