Journal of Computational Physics **163,** 529–546 (2000)
doi:10.1006/jcph.2000.6584, available online at http://www.idealibrary.com on IDEAL®

Identification of Multilayered Particles from Scattering Data by a Clustering Method

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Received August 5, 1999; revised February 7, 2000

A multilayered particle is illuminated by plane acoustic or electromagnetic waves of one or several frequencies. We consider the inverse scattering problem for the identification of the layers and of the refraction coefficients of the scatterer in a non-Born region of scattering. Local deterministic and global probabilistic minimization methods are studied. A special reduction procedure is introduced to reduce the dimensionality of the minimization space. Deep's and the multilevel single-linkage methods for global minimization are used for the solution of the inverse problem. Their performance is analyzed for various multilayer configurations.

Key Words: inverse scattering; global minimization; clustering method.

1. INTRODUCTION

Many practical problems require identification of the internal structure of an object given some measurements of its surface. In this paper we study such identification for a multilayered particle illuminated by acoustic or electromagnetic plane waves. Thus, the problem discussed here is an inverse scattering problem. A similar problem for the particle identification from the light scattering data is studied in [29]. The precise formulation of the problem is postponed until Section 2. Our approach is to reduce the inverse problem to the best fit to data multidimensional minimization. This is done in Section 3. It is also shown there that more than one frequency of the incoming waves is required to provide a stable identification. The resulting minimization is a challenging problem, since the objective function has many narrow local minima. Finding a global minimum (the sought identification) is the main subject of the study here. In Section 4 we analyze various local minimization methods and develop a special local minimization method. This method, together with a specially designed reduction procedure, is capable of finding this type of local minima. In Section 5 Kan and Timmer's multilevel single-linkage method for global minimization is presented.

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Its pairing with the local minimization method of Section 4, finally, gives the tool for the successful scatterer's identification. A detailed numerical evidence of the performance of this method is presented in Section 6.

2. DIRECT PROBLEM

Let $D \subset \mathbb{R}^2$ be the circle of a radius $R > 0$,

$$D_m = \{x \in \mathbb{R}^2 : r_{m-1} < |x| < r_m, \quad m = 1, 2, \ldots, N\} \tag{2.1}$$

and $S_m = \{x \in \mathbb{R}^2 : |x| = r_m\}$ for $0 = r_0 < r_1 < \cdots < r_N < R$. Suppose that a multilayered scatterer in D has a constant refractive index n_m in the region D_m, $m = 1, 2, \ldots, N$. If the scatterer is illuminated by a plane harmonic wave, then, after the time dependency is eliminated, the total field $u(x) = u_i(x) + u_s(x)$ satisfies the Helmholtz equation

$$\Delta u + k_0^2 u = 0, \quad |x| > r_N, \tag{2.2}$$

where $u_i(x) = e^{ik_0 x \cdot \alpha}$ is the incident field and α is the unit vector in the direction of propagation. The scattered field u_s is required to satisfy the Sommerfeld radiation condition at infinity; see [8].

Let $k_m^2 = k_0^2 n_m$. We consider the following transmission problem,

$$\Delta u_m + k_m^2 u_m = 0, \quad x \in D_m, \tag{2.3}$$

under the assumption that the fields u_m and their normal derivatives are continuous across the boundaries S_m, $m = 1, 2, \ldots, N$.

In fact, the choice of the boundary conditions on the boundaries S_m depends on the physical model under consideration. The above model may or may not be adequate for an electromagnetic or acoustic scattering, since the model may require additional parameters (such as the mass density and the compressibility) to be accounted for. However, since the goal of this paper is to study algorithms capable of resolving the inverse scattering problem, we will accept the above simplified problem here. For more details on transmission problems, including the questions on the existence and the uniqueness of the solutions, see [1, 13, 27].

The inverse problem to be solved is:

IPS. Given $u(x)$ for all $x \in S = \{x : |x| = R)$ at a fixed $k_0 > 0$, find the number N of the layers, the location of the layers, and their refractive indices n_m, $m = 1, 2, \ldots, N$ in (2.3).

Here IPS stands for a single-frequency inverse problem. Numerical experience shows that there are some practical difficulties in the successful resolution of the IPS even when no noise is present. While there are some results on the uniqueness for the IPS (see [1]), assuming that the refractive indices are known, and only the layers are to be identified, no stability estimates are available. The identification is successful, however, if the scatterer is subjected to a probe with plane waves of several frequencies. Thus, we state the multifrequency inverse problem:

IPM. Given $u^p(x)$ for all $x \in S = \{x : |x| = R)$ at a finite number P of wave numbers $k_0^{(p)} > 0$, find the number N of the layers, the location of the layers, and their refractive indices n_m, $m = 1, 2, \ldots, N$ in (2.3).

3. BEST FIT PROFILES

If the refractive indices n_m are sufficiently close to 1, then we say that the scattering is weak. In this case the scattering is adequately described by the Born approximation, and there are methods for the solution of the above inverse problems. See [8, 9, 23, 24] for further details. However, with such as assumption is inappropriate, the preferred method is to match the given observations to a set of solutions for the direct problem. Since our interest is in the solution of the IPS and IPM in the non-Born region of scattering, we choose to follow the best fit to data approach. This approach is used widely in a variety of applied problems; see, e.g., [4].

Note that, by the assumption, the scatterer has the rotational symmetry. Thus, we only need to know the data for one direction of the incident plane wave. For this reason we fix $\alpha = 0$ in (2.2) and assume that the (complex) data functions

$$g^{(p)}(\theta), \quad p = 1, 2, \ldots, P \tag{3.1}$$

are given for $0 \le \theta < 2\pi$, corresponding to the observations measured on the surface S of the ball D for a finite set of free space wavenumbers $k_0^{(p)}$.

Fix a positive integer M. Given a configuration,

$$Q = (r_1, r_2, \ldots, r_M, n_1, n_2, \ldots, n_M), \tag{3.2}$$

we solve the direct problem (2.2)–(2.3) (for each free space wavenumber $k_0^{(p)}$) with the layers $D_m = \{x \in \mathbb{R}^2 : r_{m-1} < |x| < r_m, m = 1, 2, \ldots, M\}$, and the corresponding refractive indices n_m, where $r_0 = 0$. Let

$$w^{(p)}(\theta) = u^{(p)}(x)|_{x \in S}. \tag{3.3}$$

Fix a set of angles $\Theta = (\theta_1, \theta_2, \ldots, \theta_L)$ and let

$$\|w\|_2 = \left(\sum_{l=1}^{L} w^2(\theta_l) \right)^{1/2}. \tag{3.4}$$

Define

$$\Phi(r_1, r_2, \ldots, r_M, n_1, n_2, \ldots, n_M) = \frac{1}{P} \sum_{p=1}^{P} \frac{\left\| w^{(p)} - g^{(p)} \right\|_2^2}{\left\| g^{(p)} \right\|_2^2}, \tag{3.5}$$

where the same set Θ is used for $g^{(p)}$ as for $w^{(p)}$.

We solve the IPM by minimizing the above best fit to data functional Φ over an appropriate set of admissible parameters $A_{\text{adm}} \subset \mathbb{R}^{2M}$.

It is reasonable to assume that the underlying physical problem gives some estimate for the bounds n_{low} and n_{high} of the refractive indices n_m as well as for the bound M of the expected number of layers N. Thus,

$$A_{\text{adm}} \subset \{(r_1, r_2, \ldots, r_M, n_1, n_2, \ldots, n_M) : 0 \le r_i \le R, n_{\text{low}} \le n_m \le n_{\text{high}}\}. \tag{3.6}$$

Note that the admissible configurations must also satisfy

$$r_1 \le r_2 \le r_3 \le \cdots \le r_M. \tag{3.7}$$

As already mentioned in Section 2, the numerical evidence shows that IPS is, practically, unresolvable. Here is an example to illustrate the situation. Let the configuration Q_1 be $(0.4, 0.6, 0.49, 9.0)$ with $N = 2$ and $R = 1.0$. Thus, Q_1 corresponds to the two-layer cylinder

$$n(x) = \begin{cases} 0.49 & 0 \le x < 0.4 \\ 9.0 & 0.4 \le |x| < 0.6 \\ 1.0 & 0.6 \le |x| \le 1.0. \end{cases}$$

Let $Q_2 = (0.3794, 0.5662, 0.6377, 0.040, 8.282, 5.969)$ with $N = 3$ and $R = 1.0$; thus, Q_2 corresponds to the three-layer cylinder

$$n(x) = \begin{cases} 0.040 & 0 \le |x| < 0.3794 \\ 8.282 & 0.3794 \le |x| < 0.5662 \\ 5.969 & 0.5662 \le |x| < 0.6377 \\ 1.0 & 0.6377 \le |x| \le 1.0. \end{cases}$$

Let the data $g(\theta)$ be collected for just one wavenumber $k_0 = 3.0$. Figures 1 and 2 show the real and imaginary parts of the solutions for these two configurations. The solutions are practically indistinguishable, especially if noise is present. Letting Q_1 be the original configuration for which the data $g(\theta)$ is observed, the value of Φ at the configuration Q_2 is just 0.00012. Thus, there is no way (by any method) to determine the original configuration Q_1 of the scatterer. Clearly, there are many more configurations that would produce practically identical observations. Even if it could be proven that, theoretically, there is a unique

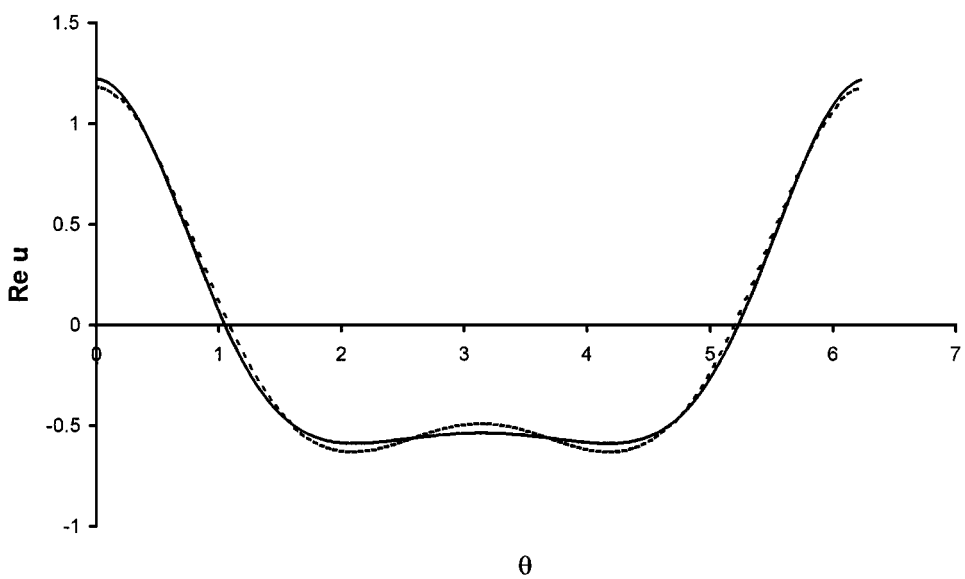

FIG. 1. Real part of the solutions for configurations Q_1 (solid line) and Q_2 on the circle S for $k_0 = 3$, $\Phi(Q_2) = 0.00012$.

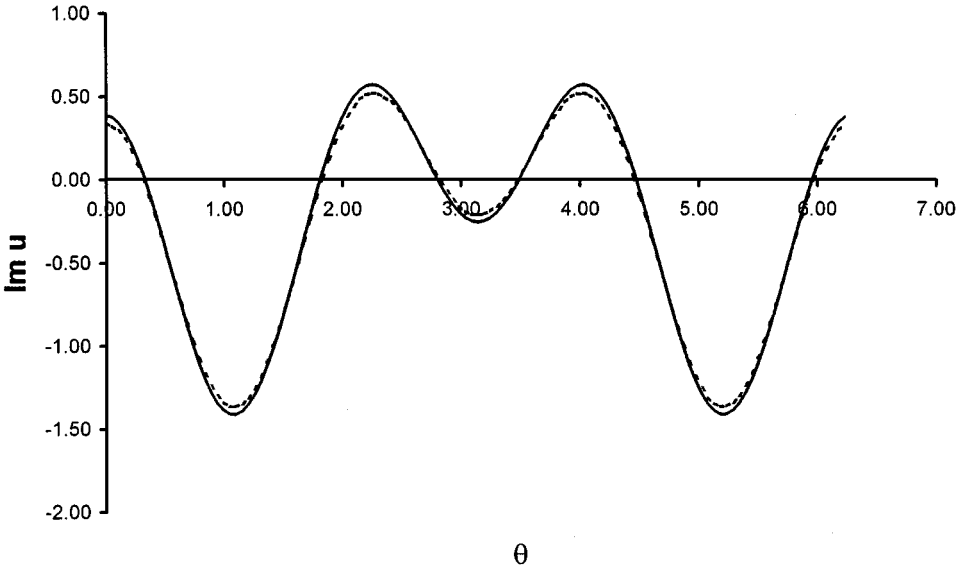

FIG. 2. Imaginary part of the solutions for configurations Q_1 (solid line) and Q_2 on the circle S for $k_0 = 3$, $\Phi(Q_2) = 0.00012$.

solution for this IPS, it would be useless in practice, because of this and other practically undistinguishable configurations.

On the other hand, the situation is quite different if we allow the scatterer to be probed with waves of multiple frequencies.

Figures 3 and 4 show the real and imaginary parts for the same configurations Q_1 and Q_2 when the free space wavenumber k_0 is equal to 10.0. Then $\Phi(Q_2) = 1.4307$. It is, of course,

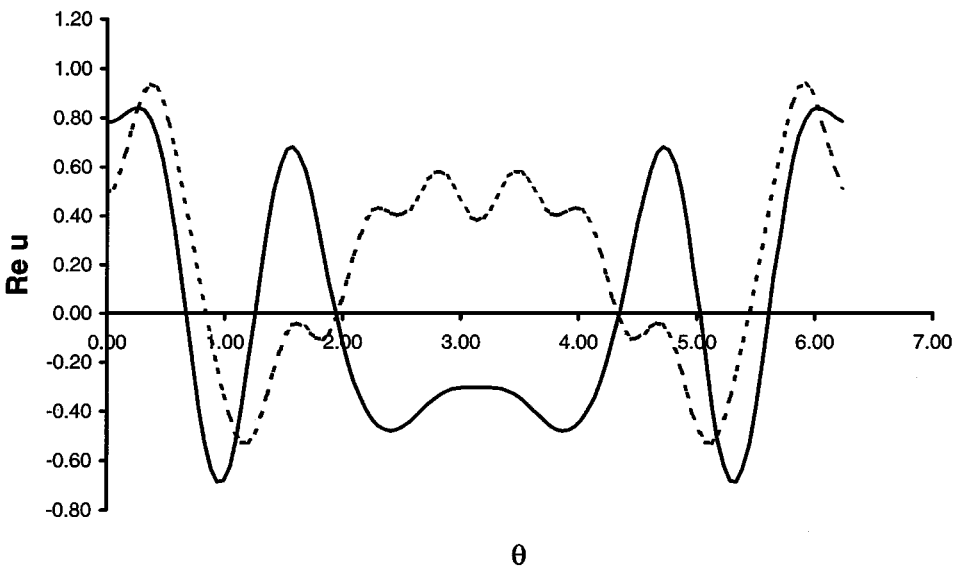

FIG. 3. Real part of the solutions for configurations Q_1 (solid line) and Q_2 on the circle S for $k_0 = 10$, $\Phi(Q_2) = 1.4307$.

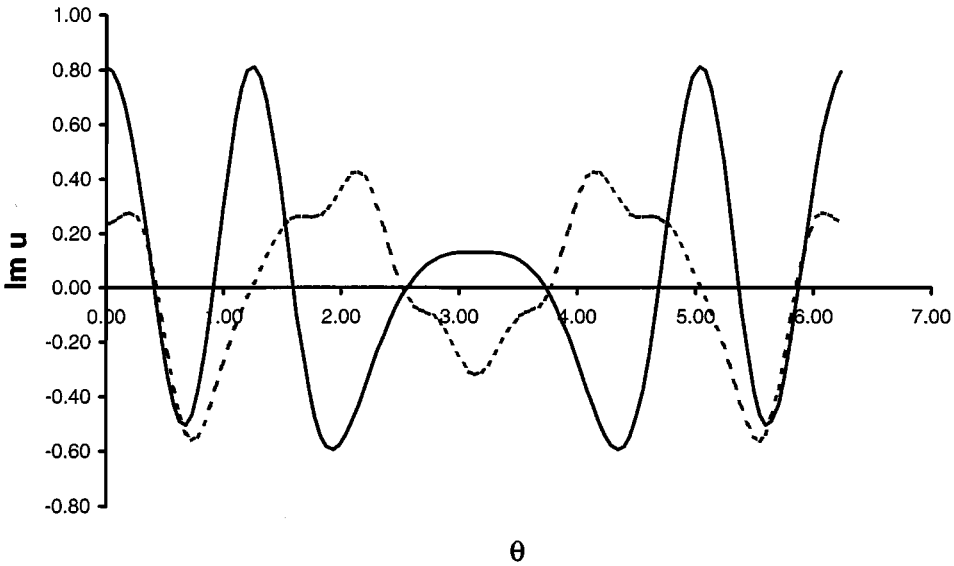

FIG. 4. Imaginary part of the solutions for configurations Q_1 (solid line) and Q_2 on the circle S for $k_0 = 10$, $\Phi(Q_2) = 1.4307$.

possible that there are configurations undistinguishable at this frequency, but combining the output for several frequencies, we can hope to achieve a reasonable recovery of the original scatterer. We show in the subsequent sections, that it is, indeed, the case. While there are many theoretical questions concerning the best or a reasonable choice of frequencies, uniqueness for the IPM, stability estimates, etc., this work indicates the practicality of the multifrequency approach.

To illustrate this point further, let P be the set of three free space wavenumbers $k_0^{(p)}$ chosen to be

$$P = \{3.0, 6.5, 10.0\}. \tag{3.8}$$

Figure 5 shows the profile of the functional Φ as a function of the variable r, $0.1 \le r \le 0.6$, in the configurations q_r with

$$n(x) = \begin{cases} 0.49 & 0 \le |x| < r \\ 9.0 & r \le |x| < 0.6 \\ 1.0 & 0.6 \le |x| \le 1.0. \end{cases}$$

The best fit to data functional exhibits a sharp minimum at $r = 0.4$; thus, there is hope to identify the sought configuration.

4. LOCAL MINIMIZATION METHODS

Using the best fit to data functional Φ defined in (3.5), the IPM is reduced to a restrained minimization over the admissible set A_{adm}, defined in (3.6) and (3.7). It is well-known that a multidimensional minimization is an extremely difficult problem, unless the objective function is "well behaved." The most important quality of such a cooperative function is

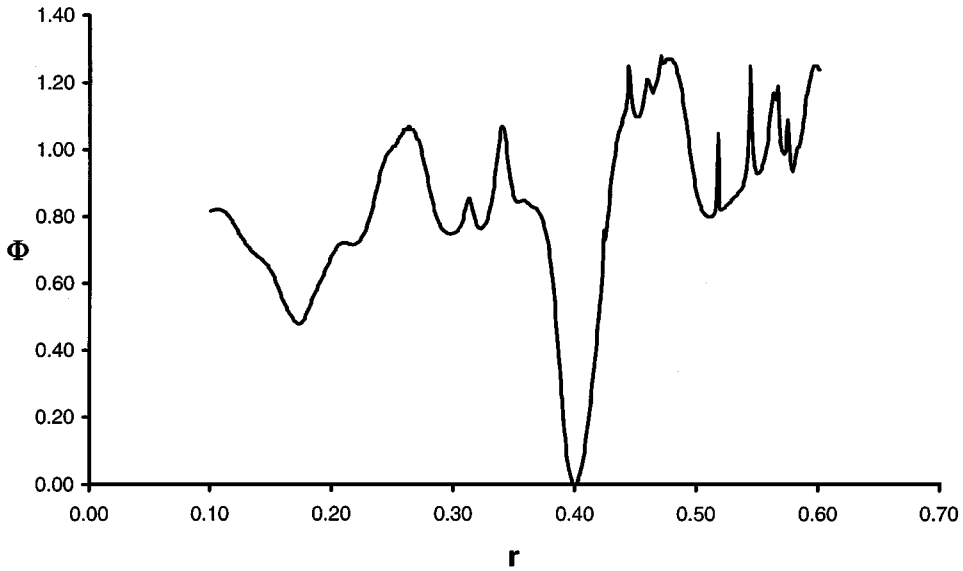

FIG. 5. Best fit profile for the configurations q_r; multiple frequencies $P = \{3.0, 6.5, 10.0\}$.

the presence of just a few local minima. Unfortunately, this is, decidedly, not the case in many applied problems and, in particular, for the problem under the consideration.

Figure 5 shows that our objective function Φ has many local minima even along this arbitrarily chosen one-dimensional cross-section of the admissible set. There are sharp peaks and large gradients. Consequently, the gradient-based methods (see [7, 11, 14, 17, 19, 22]) would not be successful for a significant portion of this region. It is also appropriate to notice that the dependency of Φ on its arguments is highly nonlinear. Thus, the gradient computations must be done numerically, which makes them computationally expensive. More importantly, the gradient-based minimization methods (as expected) perform poorly for these problems. These complications are avoided by considering conjugate gradient-type algorithms which do not require the knowledge of the derivatives at all. One such method is the Powell's method.

For an N-dimensional space the method can be described as follows (see [7]).

Powell's Method

1. Initialize the set of directions u_i to the basis vectors

$$u_i = e_i, \quad i = 1, 2, \ldots, N.$$

2. Save the starting position as Q_0.
3. For $i = 1, \ldots, N$ move Q_{i-1} to be minimum along the direction u_i and call this point Q_i.
4. For $i = 1, \ldots, N$, set $u_i = u_{i-1}$.
5. Set $u_N = P_N - P_0$.
6. Move P_N to the minimum along direction u_N and call this point P_0.

It can be shown that an iteration of this procedure produces a set u_i of mutually conjugate directions, provided, as usual, that the objective function is quadratic. It also implies a

quadratic convergence for nearly quadratic functions. The main difficulty here is that the obtained set of conjugate directions tends to become "folded up," that is, linearaly dependent. However, as noted in [7], the set of directions u_i can be reset to the basis vectors e_i after every N or $N+1$ iterations of the basic procedure.

As explained in the next section, we leave the global exploration of the admissible set to global minimization methods. A local minimization is used to explore an immediate vicinity of the initial configuration $Q \in \mathbb{R}^{2M}$. With this goal in mind, given a configuration $Q \in \mathbb{R}^{2M}$ and a direction u in $\mathbb{R}^{2M}$ we seek a minimum of Φ along this direction (by a bisection or a Golden Rule method) by restricting the probed points (at every minimization step) to the admissible set and by keeping them within a certain distance from the initial minimization point. This distance $d_{\min}$ is determined a priori to be a percentage of the characteristic length of A_{adm}.

More precisely, the "turtle" one-dimensional minimization is done as follows.

One-Dimensional Minimization

1. Let the starting position be Q_0.
2. Move from Q_0 along the given direction u by the distance $d_{\min}$ to obtain $Q_1 \in A_{\text{adm}}$.
3. Find the minimum of Φ on the interval $[Q_0, Q_1]$.

If the minimum is attained inside the interval, then stop.
If the minimum is attained at Q_0, then reverse the direction.
If the minimum is attained at Q_1, then rename $Q_0 = Q_1$, and repeat the procedure.

We have used Brent's minimization method [7] for the one-dimensional minimization in the step 3. This way the local minimum clesest (the resolution is set up by $d_{\min}$) to the starting configuration Q_0 is determined. The choice of $d_{\min}$ must be balanced between the desire to explore the fine structure of the objective function and the computational costs.

Now we can describe our basic local minimization method in $\mathbb{R}^{2M}$. The above "turtle" one-dimensional minimization procedure is used in all the minimization steps below.

Basic Local Minimization Method

1. Initialize the set of directions u_i to the basis vectors

$$u_i = e_i, \quad i = 1, 2, \ldots, 2M.$$

2. Save the starting position as Q_0.
3. For $i = 1, \ldots, 2M$ move from Q_0 along the direction u_i to find the point of minimum Q_i^t.
4. Reindex the direction u_i, so that (for the new indices) $\Phi(Q_1^t) \le \Phi(Q_2^t) \le, \ldots, \Phi(Q_{2M}^t) \le \Phi(Q_0)$.
5. For $i = 1, \ldots, 2M$ more Q_{i-1} to the minimum along the direction u_i and call this point Q_i.
6. Set $v = Q_{2M} - Q_0$.
7. Move Q_{2M} to the minimum along direction v and call this point Q_0.
8. Repeat the above steps until a stopping criterion is satisfied.

Note that we use the temporary points of minima Q_i^t only to rearrange the initial directions u_i in a different order. This method falls within the category of the Powell

minimization methods and, as mentioned above, produces conjugate directions and a quadratic convergence for nearly quadratic functions.

Still another refinement of the above algorithm has turned out to be necessary to produce a successful minimization. Since the dimension $2M$ of the minimization space was chosen a priori to be larger than $2N$, where N is the (unknown) number of layers in the original scatterer, we expect that the sought point of minimum will be located in a lower-dimensional subspace of the minimization space $\mathbb{R}^{2M}$. This information available from the specific structure of our minimization problem appears to be nontrivial. Suffice it to say, that all of our numerical experiments described in Section 6 have failed without the following (space dimension) "reduction" procedure. The main idea behind it is to conduct the local minimization searches in as low-dimensional subspaces as possible. It is specific to the inverse scattering problem for multilayer scatterer.

If two adjacent layers have close refraction coefficients in the sense that the objective functional Φ is not changed much when the two layers are assigned the same refraction coefficient, then these two layers can be replaced with just one occupying their place. The minimization problem becomes constrained to a lower-dimensional subspace of $\mathbb{R}^{2M}$ and the local minimization is done in this subspace. A similar procedure was used by us in [15] for the search of small subsurface objects.

Reduction Procedure

Let ϵ_r be a positive number.

1. Save the starting configuration $Q_0 = (r_1, r_2, \dots, r_M, n_1, n_2, \dots, n_M)$ and $\Phi(Q_0)$. Let the $(M+1)$st layer be $D_{M+1} = \{r_M \le |x| \le R\}$ and $n_{M+1} = k_0^2$.
2. For $i = 2, \dots, M+1$ replace n_{i-1} in the layer D_{i-1} by n_i. Compute Φ at the new configuration Q_i^d, and the difference $c_i^d = |\Phi(Q_0) - \Phi(Q_i^d)|$.
3. For $i = 1, \dots, M$ replace n_{i+1} in the layer D_{i+1} by n_i. Compute Φ at the new configuration Q_i^u, and the difference $c_i^u = |\Phi(Q_0) - \Phi(Q_i^u)|$.
4. Find the smallest among the numbers c_i^d and c_i^u. If this number is less than $\epsilon_r \Phi(Q_0)$, adjust the refraction coefficient to n_i in the "down" or "up" layer accordingly. Replace the two adjacent layers with one occupying their place, and renumber the layers.
5. Repeat the above steps until no further reduction in the number of layers is occurring.

Note that an application of the reduction procedure may or may not result in the actual reduction of layers.

Finally, the entire local minimization method (LMM) consists of the following:

Local Minimization Method (LMM)

1. Let the starting configuration be $Q_0 = (r_1, r_2, \dots, r_M, n_1, n_2, \dots, n_M)$.
2. Apply the reduction procedure to Q_0, and obtain a reduced configuration Q_0^r containing M^r layers.
3. Apply the basic minimization method in $A_{\text{adm}} \cap \mathbb{R}^{2M^r}$ with the starting point Q_0^r, and obtain a configuration Q_1.
4. Apply the reduction procedure to Q_1, and obtain a final reduced configuration Q_1^r.

5. GLOBAL MINIMIZATION METHODS

Given an initial configuration Q_0 a local minimization method finds a local minimum near Q_0. On the other hand, global minimization methods explore the entire admissible set to find a global minimum of the objective function. While the local minimization is usually deterministic, the majority of the global methods are probabilistic in their nature. There are great interest and activity in the development of efficient global minimization methods; see. e.g. [4, 6]. Among them are the simulated annealing method ([20, 21]), various genetic algorithms [16], interval method, and the TRUST method ([2, 3]). As we have already mentioned, the best fit to data functional Φ has many narrow local minima. In this situation it is exceedingly unlikely to get the minima points by chance alone. Thus, our special interest is in the minimization methods, which combine a global search with a local minimization. In [15] we developed such a method (the hybrid stochastic-deterministic method) and applied it to the identification of small subsurface particles, provided a set of surface measurements. The HSD method could be classified as a variation of a genetic algorithm with a local search with reduction. In this paper we consider the performance of two algorithms: Deep's method and Kan and Timmer's multilevel single-linkage method. Both combine a global and a local search to determine a global minimum. Recently, these methods have been applied to a similar problem of the identification of particles from their light scattering characteristics in [29]. Unlike [29], our experience shows that Deep's method has failed consistently for the type of problems we are considering. See [10, 29] for more details on Deep's method.

Multilevel Single-Linkage Method (MSLM)

Kan and Timmer [25, 26] give a detailed description of this algorithm. Zakovic *et al.* in [29] describe in detail an experience of its application to an inverse light scattering problem. They also discuss different stopping criteria for the MSLM. Thus, we give here only a shortened and an informal description of this method and of its algorithm.

In a pure *random search* method a batch H of L trial points is generated in A_{adm} using a uniformly distributed random variable. Then a local search is started from each of these L points. A local minimum with the smallest value of Φ is declared to be the global one.

A refinement of the random search is the *reduced sample random search* method. Here we use only a certain fixed fraction $\gamma < 1$ of the original batch of L points to proceed with the local searches. This reduced sample H_{red} of γL points is chosen to contain the points with the smallest γL values of Φ among the original batch. The local searches are started from the points in this reduced sample.

Since the local searches dominate the computational costs, we would like to initiate them only when it is truly necessary. Given a critical distance d we define a cluster to be a group of points located within the distance d of each other. Intuitively, a local search started from the points within a cluster should result in the same local minimum, and, therefore, should be initiated only once in each cluster.

Having tried all the points in the reduced sample we have information on the number of local searches performed and the number of local minima found. This information and the critical distance d can be used to determine a statistical level of confidence that all the local minima have been found. The algorithm is terminated (a stopping criterion is satisfied) if an a priori level of confidence is reached.

If, however, the stopping criterion is not satisfied, we perform another iteration of the MSLM by generating another batch of L trial points. Then it is combined with the previously generated batches to obtain an enlarged batch H^j of jL points (at iteration j), which leads to a reduced sample H^j_{red} of γjL points. The critical distance d is reduced to d_j (thus, the cluster's size is redefined), a local minimization is attempted once within each cluster, the information on the number of local minimizations performed and the local minima found is used to determine if the algorithm should be terminated, etc.

The following is an adaptation of the MSLM method to the inverse scattering problem presented in Sections 2 and 3, with all the relevant notations. The LMM local minimization method introduced in the previous section is used here to perform local searches.

MSLM (at Iteration j)

1. Generate another batch of L trial points (configurations) from a random uniform distribution in A_{adm}. Combine it with the previously generated batches to obtain an enlarged batch H^j of jL points.

2. Reduce H^j to the reduced sample H^j_{red} of γjL points, by selecting the points with the smallest γjL values of Φ in H^j.

3. Calculate the critical distance d_j by

$$d_j^r = \pi^{-1/2}\left(\Gamma\left(1+\frac{M}{2}\right)R^M\frac{\sigma \ln jL}{jL}\right)^{1/M},$$

$$d_j^m = \pi^{-1/2}\left(\Gamma\left(1+\frac{M}{2}\right)(n_{\text{high}}-n_{\text{low}})^M\frac{\sigma \ln jL}{jL}\right)^{1/M}.$$

$$d_j = \sqrt{\left(d_j^r\right)^2+\left(d_j^n\right)^2}$$

4. Order the sample points in H^j_{red} so that $\Phi(Q_i) \le \Phi(Q_{i+1})$, $i = 1, 2, \ldots, \gamma jL$. For each value of i, start the local minimization from Q_i, unless there exists an index $k < i$, such that $\|Q_k - Q_i\| \le d_j$. Ascertain if the result is a known local minimum.

5. Let K be the number of local minimizations performed, and let W be the number of different local minima found. Let

$$W_{\text{tot}} = \frac{W(K-1)}{K-W-2}.$$

The algorithm is terminated it

$$W_{\text{tot}} < W + 0.5. \tag{5.1}$$

Here Γ is the gamma function, and σ is a fixed constant.

A related algorithm (the mode analysis) is based on a subdivision of the admisible set into smaller volumes associated with local minima. This algorithm is also discussed in [25, 26]. From the numerical studies presented there, the authors deduce their preference for the MSLM.

6. NUMERICAL RESULTS

Introducing polar coordinates in (2.3) and separating the variables, equations for the total field $u(x)$ become

$$u_1(x) = \sum_{l=-\infty}^{\infty} a_{1,l} J_l(k_1|x|)e^{il\theta}$$

for $x \in D_1$,

$$u_m(x) = \sum_{l=-\infty}^{\infty} (a_{m,l} J_l(k_m|x|) + b_{m,l} Y_l(k_m|x|))e^{il\theta}$$

for $x \in D_l$, $l = 2, \ldots, N$, and

$$u(x) = e^{ik\langle x,v\rangle} + \sum_{l=-\infty}^{\infty} A_l H_l^{(1)}(k_0|x|)e^{il\theta}$$

for $x \in D : r_N \le |x| \le R$. Here J_l, Y_l are the Bessel functions of the first and second kind, $H_l^{(1)}$ is the Hankel function of the first kind, and v is the direction vector of the incident wave. Since

$$e^{ik\langle x,v\rangle} + \sum_{l=-\infty}^{\infty} i^l J_l(k_0|x|)e^{il\theta}$$

for $v = (1, 0)$, the above equations and the conditions of continuity form a system of equations from which the field $u(x)$ can be calculated on the circle S. This solves the direct problem (2.2)–(2.3). Other methods of solution for such problems are known as well; see, e.g., [18, 28]. Solving the direct problem for the set P of three free wave numbers $k_0^{(p)}$ (see (3.8)), we obtain the total fields $u^{(p)}(x)$. Their restrictions to S give the (simulated) data $g^{(p)}(\theta)$.

Our approach to the inverse problem IPM (see Section 2) is to recast it in the best fit to data form (3.5) and to minimize the objective functional Φ over A_{adm}. We have tested Deep's global minimization method, the multilevel single-linkage method, and a reduced sample random search method. Each method was tried for three different original configurations Q_0 described below. The data $g^{(p)}(\theta)$ was computed at 120 angles $\theta_l = 2\pi l/120$, $l = 1, 2, \ldots, 120$, and Φ was evaluated according to (3.4) and (3.5). This data was used with three different noise levels $\delta = 0.00$, 0.03, and 0.10. More precisely, for the uniformly distributed on [0, 1] random variable z

$$g_\delta(\theta) = g(\theta) + \delta\|g\|(2z - 1)(1 + i)$$

for the noise level δ.

Since our goal was to test the applicable algorithms, the values for the refraction coefficients, the size, the wavenumbers, etc., were chosen arbitrarily at this time, that is, without a regard for their possible physical relevancy. The original configurations are:

Configuration $Q_0^{(1)}$. This is a one-layer cylinder $Q_0^{(1)} = (0.72, 4.2025)$ with $N = 1$ and $R = 1.0$; see (3.2). That is, the refraction coefficient is defined by

$$n(x) = \begin{cases} 4.2025 & 0 \le |x| < 0.72 \\ 1.0 & 0.72 \le |x| \le 1.0. \end{cases}$$

Configuration $Q_0^{(2)}$. This is a two-layer cylinder $Q_0^{(2)} = (0.4, 0.6, 0.49, 9.0)$ with $N = 2$ and $R = 1.0$; that is,

$$n(x) = \begin{cases} 4.49 & 0 \le |x| < 0.4 \\ 9.0 & 0.4 \le |x| < 0.6 \\ 1.0 & 0.6 \le |x| \le 1.0. \end{cases}$$

Configuration $Q_0^{(3)}$. This is a three-layer cylinder $Q_0^{(3)} = (0.3, 0.7, 0.8, 4.0, 25.0, 9.0)$ with $N = 3$ and $R = 1.0$; that is,

$$n(x) = \begin{cases} 4.0 & 0 \le |x| < 0.3 \\ 25.0 & 0.3 \le |x| < 0.7 \\ 9.0 & 0.7 \le |x| < 0.8 \\ 1.0 & 0.8 \le |x| \le 1.0. \end{cases}$$

To identify these configurations we applied the global minimization methods of Section 5. In each one we let $M = 4$, $R = 1.0$. A priori bounds for the refraction coefficients were chosen to be $n_{\text{low}} = 0.04$ and $n_{\text{high}} = 30.25$. Minor modifications to the description of the methods in Section 5 were introduced for the purpose of computational simplification. In particular, the minimization was done in $\sqrt{n_m}$ rather than in n_m as stated there. This results in a rescaling of the admissible set. In each case, after a global minimum $Q_{\min}$ was determined, the error of the identification

$$\epsilon_{\text{err}} = \frac{\int_D |n_{\min}(x) - n(x)|}{\int_D n(x)}, \tag{6.1}$$

where $n(x)$ is the refraction coefficient of the original configuration Q_0, was computed to determine if the identification was successful. We distinguished between the two levels of a successful identification: $\epsilon_{\text{err}} < 0.01$ and $\epsilon_{\text{err}} < 0.1$.

Identification by Deep's Method [10, 29]

Each test of the method consisted of 100 independent runs. Since $M = 4$ the minimization was done in $\mathbb{R}^8$. As we have already mentioned, the method failed every time. It seems that the local minimization phase of Deep's method (minimization over randomly selected parabolas) is not extensive enough to identify narrow local minima present in this problem. Also, the method does not use the reduction procedure (see Section 4), which, we think, is another reason for its failure. As in [29] we have also observed the cycling of the algorithm.

Identification by Reduced Sample Random Search Method

This method is presented in Section 5 in the subsection on the multilevel single-linkage method. The local minimization method with the reduction procedure (as described in

TABLE I
Identification by MSLM

Noise	Runs	Success rate[a] 0.01	0.1	Smallest Φ
$\delta = 0.00$	10	8	10	0.0000
$\delta = 0.03$	10	9	10	0.0016
$\delta = 0.10$	10	10	10	0.0178

Note. Original Configuration $Q_0^{(1)}$.
[a] Identification is successful if $\epsilon_{\text{err}} < 0.01$, or $\epsilon_{\text{err}} < 0.1$ correspondingly; see (6.1).

Section 4) was used in the local minimization phase. Chosen parameters $L = 15000$ and $\gamma = 0.01$ the performance of this method are the same, as those in the multilevel single-linkage method. In fact, $L = 15000$ is exactly the sample size in MSLM at it termination in our experiments. Since MSLM has the great advantage of a self-contained statistical stopping criteria (and from which the number 15,000 was determined in the first place), it is clearly a preferred method.

Identification by Multilevel Single-Linkage Method

We have attempted to identify all 3 original configurations, $Q_0^{(1)}$, $Q_0^{(2)}$, and $Q_0^{(3)}$, each with no noise in the data ($\delta = 0.00$) as well as with noise levels $\delta = 0.03$ and $\delta = 0.10$. See Tables I–III. Each of the 9 tests consisted of 10 independent runs. It took about 60 to 80 min on average to complete one run on a 333-MHz PC. We used $M = 4$, $R = 1.0$, $\gamma = 0.01$, and the sample size $L = 200$. The parameter σ was chosen to be equal to 1.0. Value $\sigma = 4.0$ was used in [26], and $\sigma = 1.9$ in [12]. As in Deep's method above, a priori bounds for the refraction coefficients were chosen to be $n_{\text{low}} = .04$ and $n_{\text{high}} = 30.25$. The value $\epsilon_r = 0.1$ was used in the reduction procedure (see Section 4) during the local minimization phase.

As in other work on the clustering algorithm, we have found the stopping rule (5.1) to be unsatisfactory. In our experience the difference $W_{\text{tot}} - W$, while slightly decreasing with the number of performed minimizations, has quickly stabilized around the value of 5. Thus, the stopping criterion (5.1)

$$W_{\text{tot}} < W + 0.5$$

TABLE II
Identification by MSLM

Noise	Runs	Success rate[a] 0.01	0.1	Smallest Φ
$\delta = 0.00$	10	10	10	0.0000
$\delta = 0.03$	10	1	10	0.0034
$\delta = 0.10$	10	2	9	0.0362

Note. Original Configuration $Q_0^{(2)}$.
[a] See Table I.

TABLE III
Identification by MSLM

Noise	Runs	Success rate[a] 0.01	Success rate[a] 0.2	Smallest Φ
$\delta = 0.00$	10	2	7	0.0000
$\delta = 0.03$	10	0	5	0.0071
$\delta = 0.10$	10	0	5	0.0541

Note. Original Configuration $Q_0^{(3)}$.
[a] See Table I.

could not be attained. This issue has been discussed in Refs. [5, 12], where a different stopping rule was suggested for functions with large numbers of local minima. Since the Bayesian stopping rule reflects the level of confidence in finding all the local minima, a relaxation of (5.1) would mean a lower level of confidence, which still may be acceptable to ensure that the global minimum is found among already performed local minimizations. We have chosen to replace (5.1) with

$$W_{\text{tot}} < W + 0.5 \quad \text{or} \quad W_{\text{tot}} < (1 + \epsilon_{\text{tot}})W, \tag{6.2}$$

where $\epsilon_{\text{tot}} = 0.03$.

As before

$$W_{\text{tot}} = \frac{W(K-1)}{K - W - 2},$$

where K is the number of local minimizations performed, and W is the number of different local minima found. Thus, the MSLM algorithm is terminated if (6.2) is satisfied. In our numerical experiments we have obtained the average values $K = 5000$, $W = 150$, and $W_{\text{tot}} = 155$.

An example of successful ($\epsilon_{\text{err}} < 0.1$) identification for $Q_0^{(2)}$ and $\delta = 0.10$ is shown in Fig. 6. The identified configuration is a two-layer cylinder

$$Q_{\text{id}} = (0.3966, 0.5943, 0.4684, 9.203),$$

with $\Phi(Q_{\text{id}}) = 0.0367$, $\epsilon_{\text{err}} = 0.0480$. That is,

$$n(x) = \begin{cases} 0.4684 & 0 \le |x| < 0.3966 \\ 9.203 & 0.3966 \le |x| < 0.5943 \\ 1.0 & 0.5943 \le |x| \le 1.0. \end{cases}$$

An example of a successful ($\epsilon_{\text{err}} < 0.1$) identification for $Q_0^{(3)}$ and $\delta = 0.03$ is a three-layer cylinder,

$$Q_{\text{id}} = (0.3030, 0.7067, 0.8079, 4.071, 24.528, 8.857),$$

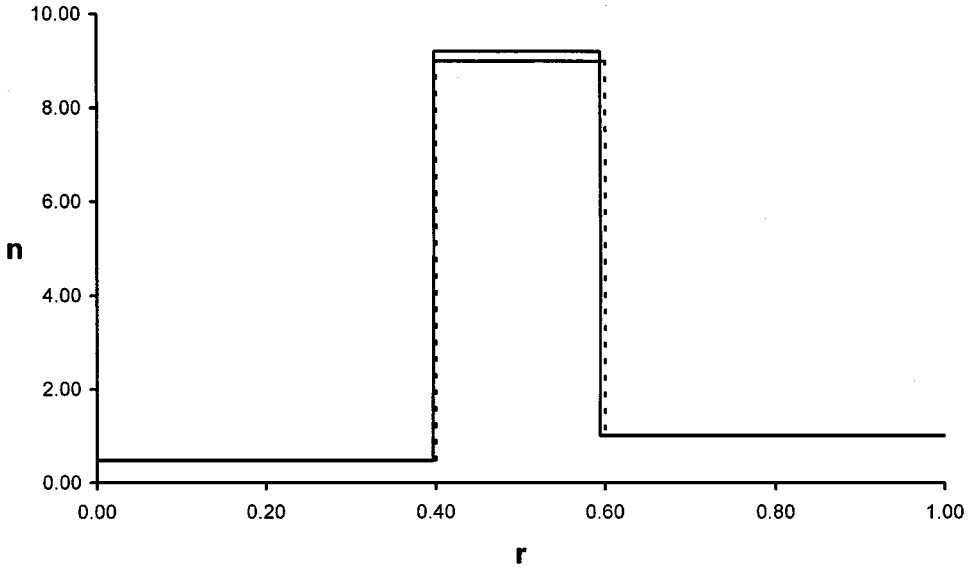

FIG. 6. Refraction coefficients $n(x)$ for the original $Q_0^{(2)}$ and the identified Q_{id} (solid line) configurations. Data noise level $\delta = 0.10$, $\Phi(Q_{\mathrm{id}}) = 0.0367$, $\epsilon_{\mathrm{err}} = 0.0480$.

with $\Phi(Q_{\mathrm{id}}) = 0.00708$, $\epsilon_{\mathrm{err}} = 0.4125$. That is,

$$n(x) = \begin{cases} 4.071 & 0 \le |x| < 0.3030 \\ 24.528 & 0.3030 \le |x| < 0.7067 \\ 8.857 & 0.7067 \le |x| < 0.8079 \\ 1.0 & 0.8079 \le |x| \le 1.0. \end{cases}$$

7. CONCLUSIONS

The inverse scattering problem IPM is the identification of a multilayered scatterer by a set of observations on its boundary. Such problems have applications in science and engineering. In the case of the week scattering approximation, many such problems can be solved by a linearized inversion. However, if the scattering is not weak, other methods of solution need to be developed. We have illustrated in Section 3 that an inversion based on just one frequency of the incident waves cannot be successful, since there are distinct configurations, producing practically the same observations. Introducing multiple frequencies, however, makes the inverse problem more amenable to a solution.

In this paper the inverse problem is transformed into the best fit to data minimization problem. This minimization is difficult, since the objective function is rugged and has many narrow local minima. A promising way to treat such a minimization is by a combination of global (probabilistic) and local (deterministic) minimization methods. In this paper we examined various local and global methods. Concerning the local minimization methods it was shown that the local minimization method (LMM) of Section 4 was successful, even when other considered methods failed. This method is a variation of a conjugate directions method with no use of partial derivatives. It has a quadratic convergence near quadratically shaped minima. However, even this method needs to be enhanced by a reduction procedure

(Section 4). This procedure helps the minimization to take an advantage of the a priori available information that the sought minima are likely to be found in certain lower-dimensional subspaces of the entire minimization space.

For the global minimization part we considered Deep's method and the multilevel single-linkage method. While Deep's method failed, the MSLM was successful in many instances. It also has an important advantage of having termination criteria establishing a level of confidence that the found minima contain the sought global minimum. Among the deficiencies of the MSLM are its slow execution and inconsistency and failure to identify some configurations. There is still a problem in choosing an appropriate stopping rule. Thus, the MSLM provides a benchmark against which the performance other methods can be judged and measured.

ACKNOWLEDGMENT

I thank the referees for their valuable suggestions.

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