Solution of the inverse scattering problem by T-matrix completion

Howard W. Levinson
Department of Mathematics, University of Pennsylvania, Philadelphia, Pennsylvania 19104

Vadim A. Markel
Departments of Radiology and Bioengineering and Graduate Group in Applied Mathematics and Computational Science, University of Pennsylvania, Philadelphia, Pennsylvania 19104

Abstract. We propose a conceptually new method for solving nonlinear inverse scattering problems (ISPs). The method is inspired by the theory of nonlocality of physical interactions and utilizes the relevant mathematical formalism. We formulate the ISP as a problem whose goal is to determine an unknown interaction potential $V$ from external scattering data. We then utilize the one-to-one correspondence between $V$ and the T-matrix of the problem, $T$. An iterative process is formulated for the T-matrix in which we seek $T$ that is (i) compatible with the data and (ii) corresponds to an interaction potential $V$ that is as diagonally-dominated as possible but not necessarily strictly diagonal. We refer to this algorithm as to the data-compatible T-matrix completion (DCTMC).

1. Introduction

Most inverse scattering problems (ISPs) are known to be nonlinear [1,2]. This is so because the superposition principle is rarely applicable to the physical parameters that one seeks to reconstruct in an ISP. For example, in linear electrodynamics, the fields created by two separate sources of radiation are given by the sum of fields produced by each source separately. However, the fields scattered by two objects are not, generally, equal to the sum of fields scattered by each of them separately, unless the objects are placed sufficiently far apart so that multiple scattering can be ignored. If we wish to reconstruct the location or shape of the objects from scattering data, the problem is obviously nonlinear.

Nonlinear ISPs are abundant in tomography. Here linear problems are more or less exceptions, encountered only when monochromatic waves or particles travel through the medium along well-defined trajectories, as is the case in the conventional computerized tomography (CT) with mono-energetic X-rays. If the X-ray source has a broad energy
distribution and the medium properties are energy-sensitive, the ISP becomes nonlinear. In problems involving scattering of waves, ISPs are nonlinear as a rule.

In some cases, the nonlinearity is so severe that there is no hope to solve the ISP in practice. For instance, if an object is placed inside a strongly absorbing shell, the effect it makes on the fields scattered by the system “shell+object” is exponentially small. Unless the scattered fields are noiseless and measured with exponential precision and the forward model is exact (all fairly unrealistic assumptions), there is no hope to recover the object from external measurements. Similarly, in inverse Schroedinger scattering, there may exist “hidden parameters” associated with discrete (bound) states that are impossible to determine uniquely from scattering measurements.

However, with the use of suitable regularization, many nonlinear ISPs can be solved with reasonable precision. As a result, nonlinear ISPs continue to attract considerable attention. Such problems are encountered, for example, in optical diffusion tomography [3, 4], diffraction tomography [5, 6], electrical impedance tomography (Calderon problem) [7–9] and the near-field electromagnetic imaging [10–12]. However, solving nonlinear ISPs is a difficult numerical task, especially in three dimensions. This is even more true for problems involving large data sets that are available with the use of modern experimental techniques. Developing efficient algorithms for solving nonlinear ISPs remains an important challenge.

Nonlinear ISPs are amply reviewed in the modern literature [2, 13–16]. The mainstream approach to solving nonlinear ISPs is the iterative Newton method and its variants such as the Levenberg-Marquardt method, iteratively regularized Gauss-Newton method, Newton-Kantorovich method and steepest descent (Landweber iteration). These methods (except for Newton-Kantorovich) are succinctly explained in [17]. The Newton-Kantorovich iterations are closely related [18] to the method of inverse Born series [9,19,20]. In the context of quantum mechanics, Gel’fand-Levitan and Marchenko methods [13] are frequently used, but typically in one dimension. Also in this method the energy of incident particles is varied and it is assumed that the interaction potential is independent of energy – a justified assumption in inverse quantum scattering but not necessarily in other scattering problems where the potential of interest may depend on energy or frequency of the waves used due to the effect of dispersion. A different class of non-deterministic inversion approaches that make use of some form of prior knowledge about the reconstructed object is based on Bayesian inference [21]. The common feature of all these approaches (except for the inverse Born series) is that a certain cost function is minimized and updated iteratively and that this cost function depends on all available measurements (data points). In the case of inverse Born series, the solution is obtained as an analytically-computable functional of the data.

The method of this paper is conceptually different from the methods reviewed above and is based on a digression into a seemingly unrelated field of physics, namely, into the theory of nonlocality. This theory accounts for the fact that certain physical processes or interactions occurring at a point \( r \) in space can be influenced by the field in some finite vicinity of that point. For example, in local electrodynamics, Ohm’s law
is written as \( J(r) = \sigma(r)E(r) \). In a nonlocal theory, this linear relation is generalized by writing \( J(r) = \int V(r,r')E(r')d^3r' \). Of course, we expect on physical grounds that \( V(r,r') \rightarrow 0 \) when \( |r - r'| > \ell \), where \( \ell \) is the characteristic scale of nonlocality (the radius of influence), which is usually much smaller than the overall size of the sample. If the electric field \( E(r) \) does not change noticeably on the scale of \( \ell \), we can define the local conductivity as \( \sigma(r) = \int V(r,r')d^3r' \) and use Ohm’s law in its local form. This is all well known in physics. However, implications of nonlocality for nonlinear ISPs have not been considered so far.

Let us assume that we want to find \( \sigma(r) \) from measurements of voltage drop for a constant current injected into the sample by two point-like electrodes attached to its surface at various points (Calderon problem). It turns out that a much simpler problem is to seek a nonlocal kernel \( V(r,r') \). This statement may seem trivial because \( V(r,r') \) has more degrees of freedom than \( \sigma(r) \) but, to the best of our knowledge, this idea has not been utilized so far. Of course, it is understood that a general \( V(r,r') \) cannot be uniquely determined from a typical data set because the number of unknown parameters (degrees of freedom) in \( V \) is in this case much larger than the number of measurements. However, as explained above, we also expect that \( V(r,r') \) should be approximately diagonal. We then proceed as follows:

(i) First, we define a class of kernels \( V(r,r') \) that are compatible with the measured data. This is the only instance when the data are used and it turns out that the size of the data set is not a limiting factor for this step.

(ii) Then we iteratively reduce the off-diagonal norm of \( V \) by a process somewhat reminiscent of matrix completion. The kernel \( V \) remains within the class of “data-compatible” kernels and data are not used in the iterations.

(iii) Once the ratio of the off-diagonal and diagonal norms of \( V \) is deemed sufficiently small (we do not truly hope to reduce it precisely to zero), we compute \( \sigma(r) = \int V(r,r')d^3r' \). This gives a numerical solution to the nonlinear inverse problem. We note that in practice all operators are represented by matrices and that integration in the above formula should be replaced by column-wise summation to the diagonal.

Also, the diagonal and off-diagonal norms mentioned above are defined for matrices.

We refer to the above algorithm as to the data-compatible T-matrix completion (DCTMC). We underscore that physical interactions are never truly local and that some small degree of nonlocality exists in all physical systems. However, the radius of influence \( \ell \) is typically so small (e.g., equal to the atomic scale for the nonlocal dielectric response of most natural substances) that the nonlocality can be ignored for most practical purposes. In our approach, we relax this condition and allow \( V \) to be off-diagonal on much larger scales. Of course, we will seek to find \( V \) that is as diagonal as possible. However, we do not expect to eliminate all off-diagonal terms that are separated by more than one atomic scale (not to mention that such fine discretization of the medium is practically impossible). Thus, the non-locality of \( V \) utilized in DCTMC is not an intrinsic physical property but rather a physically-inspired mathematical trick.
that is used to simplify solution of the nonlinear ISP. In other words, we simplify the solution of the ISP by slightly relaxing the underlying physical model.

The above gives a broad idea of DCTMC. A technical description is given in Sec. 2 a nonlinear ISP arising in scalar wave imaging is described in Sec. 3 an easily-analyzable toy problem involving only two interacting scatterers is discussed in Sec. 4 and numerical results are given in Sec. 5.

2. Mathematical description of DCTMC

2.1. General formulation of the ISP

Consider a linear operator \( \mathcal{L} \) and the equation

\[
\mathcal{L}u(r) = S(r)
\]

where \( u \) is a physical field and \( S \) is the source term. Let \( \mathcal{L} = \mathcal{L}_0 - V \), where \( \mathcal{L}_0 \) is known and \( V \) is the unknown interaction operator that we seek to reconstruct. As discussed above, we assume at the outset that \( V \) is an integral operator with the kernel \( V(r, r') \) but, eventually, the computed image will be obtained as a function of \( r \) only by integrating over the second variable, that is, we are truly interested in the function \( \int V(r, r')d^3r' \). We also assume that \( V(r, r') \neq 0 \) only if \( r, r' \in \Omega \), where \( \Omega \) is a spatial region occupied by the sample. Our goal is to recover \( V \) from the measurements of \( u \) performed outside of the sample, assuming that it is illuminated by various external sources. Note that we cannot perform measurements or insert sources inside the sample (which would have greatly simplified the ISP solution if it was physically possible).

The inverse of \( \mathcal{L} \) is the complete Green’s function of the system, denoted by \( G = \mathcal{L}^{-1} \). The formal solution to (1) is then \( u = GS \). We know that \( G \) exists as long as the forward problem has a solution. This is usually the case if \( V \) is physically admissible. Likewise, the inverse of \( \mathcal{L}_0 \) is the unperturbed Green’s function, denoted by \( G_0 = \mathcal{L}_0^{-1} \). The field \( u_0 = G_0S \) is the incident field, in other words, the field that would have existed everywhere in space in the case \( V = 0 \). Nonzero interaction \( V \) gives rise to a scattered field \( u_s \), and the total field is a sum of the incident and scattered components, \( u = u_0 + u_s \). A straightforward algebraic manipulation yields the following expression for \( u_s \):

\[
u_s = G_0(\mathbb{I} - VG_0)^{-1}VG_0S \]

where \( \mathbb{I} \) is the identity operator.

A single data point \( \Phi(r_d, r_s) \) is obtained by placing a source of intensity \( S_0 \) at the location \( r_s \) and measuring the scattered field by a detector at the location \( r_d \) and then dividing the result by \( S_0 \) (the intensity is fixed for all sources). By scanning \( r_d \) and \( r_s \) on the measurement surfaces \( \Sigma_d \) and \( \Sigma_s \) outside of the sample (see illustration in Fig. 1), we measure a function of two variables \( \Phi(r_d, r_s) \), which is coupled to \( V(r, r') \) by the equation

\[
\Phi = G_0(\mathbb{I} - VG_0)^{-1}VG_0 \]
Figure 1. Illustration of the imaging geometry and equations (3) and (4). The symbols $A$, $B$ and $\Gamma$ represent matrices obtained by restricting and sampling the unperturbed Green’s function operator $G_0(r, r')$. Note that the direction of arrows corresponds to the order of arguments of $G_0$ when read from right to left.

All product and inversion operations in the above should be understood in the operator sense. The ISP can now be formulated as follows: Given a measured function $\Phi(r_d, r_s)$, where $r_d \in \Sigma_d$ and $r_s \in \Sigma_s$, find an “approximately diagonal” kernel $V(r, r')$, where $r, r' \in \Omega$. We do not need to define “approximate diagonality” precisely at this point, but in the case of matrices that are inevitably used in calculations, this requirement implies a sufficiently small ratio of the off-diagonal and diagonal norms.

It is important to note that $G_0$ in (3) is the same operator in all instances where it appears, but for the purpose of computing the operator products, its kernel $G_0(r_1, r_2)$ is differently restricted. This is illustrated graphically in Fig. 1. Thus, for the first factor $G_0$ in the right-hand side of (3), $r_1 \in \Sigma_d$ and $r_2 \in \Omega$. For the second factor (inside the brackets) $r_1, r_2 \in \Omega$. For the last factor, $r_1 \in \Omega$ and $r_2 \in \Sigma_s$. Further, in all practical implementations, the data function is sampled rather than measured continuously and the medium is voxelized. An example of discretization will be given below in Sec. 3. At this point we proceed under the assumption that (3) can be suitably discretized and, as a result, converted to a matrix equation. In the latter, it is logical to use different notations for the matrices that are obtained by different restriction and sampling of the kernel $G_0(r_1, r_2)$. Indeed, the matrices obtained in this manner are, generally, different and can even be of different size. We will denote the matrices obtained by restricting
and sampling the first, second, and last terms $G_0$ in (3) by $A$, $\Gamma$ and $B$, respectively. Then (3) take the following form:

$$\Phi = A(I - VT)^{-1}VB.$$  \hspace{1cm} (4)

In (4), the matrices $A$, $B$ and $\Gamma$ are known theoretically, $\Phi$ is measured and we seek to solve (4) for $V$.

Eq. (4) is the main nonlinear equation that is discussed in this paper. It is, in fact, very general and encompasses many different problems of imaging and tomography. The underlying physical model is encoded in the operator $G_0$ and in the matrices $A$, $B$ and $\Gamma$ that are obtained by sampling this operator. However, the general algebraic structure of (4) is the same in many different ISPs. The following two remarks about this equation can be made:

**Remark 1: Noninvertibility of $A$ and $B$.** If matrices $A$ and $B$ were invertible in the ordinary sense, the nonlinear ISP would be solvable exactly by three operations of matrix inversion. Unfortunately, $A$ and $B$ are almost never invertible. To construct $A$ and $B$ of sufficiently high rank, one needs to perform measurements inside the medium. As was noted above, this is usually impossible. The typical sizes of all matrices involved will be discussed below (see Fig. 2 and its discussion).

**Remark 2: Linearization.** In traditional approaches, one may seek a linearization of the problem by approximating the factor $(I - VT)^{-1}V$ or, possibly, by making additional transformations of (4). The simplest approach is the first Born approximation, according to which $(I - VT)^{-1}V \approx V$. Obviously, the first Born approximation is valid if $\|VT\| \ll 1$. Other linearization methods include the first Rytov and the mean-field approximations [22]. All conventional linearization approaches assume that $V$ is strictly diagonal and operate with a vector $x$ composed of the diagonal elements of $V$. Similarly, the matrix $\Phi$ is unrolled into a vector $\phi$ by a matrix operation known as vec, that is, by stacking the columns of $\Phi$ into one column-vector. The resultant equation has the form $Kx = \phi$, where $K$ is a matrix obtained by multiplying the elements of $A$ and $B$ according to the rule $K_p(n,m,t) = A_{nt}B_{nm}$. Here the index $p(n,m)$ establishes the correspondence between the element $\phi_p$ (as defined by the vec operation) and the matrix element $\Phi_{nm}$. It can be seen that the size of $K$ is much larger than the sizes of either $A$ and $B$. The difference and the associated computational complexity is the price paid for enforcing strict diagonality of $V$. We note that because of the different book-keeping models used by the traditional approaches and by the present formulation of the ISP, Eq. (4) may seem unfamiliar.

### 2.2. T-matrix and its representations; “experimental” T-matrix

The basic definition of T-matrix (which is, actually, an operator) is through the relation between the complete and unperturbed Green’s functions: $G = G_0 + G_0T G_0$. By direct
comparison with (2) we find that
\[ T = (I - VG_0)^{-1}V . \]  

We will not use different notations for the operator \( T \) and its discretized version, which is truly a matrix. Consequently, Eq. (4) can be re-written as
\[ \Phi = AT(V)B , \]  
where
\[ T(V) = (I - VT)^{-1}V . \]  

The above equation is, in fact, the matrix formulation of the forward problem. Indeed, if we know \( V \), we can use (7) to compute \( T \), and the latter gives the most general solution to the forward problem. If we know \( T \), we can predict the result of a measurement by any detector due to any source by simple matrix multiplication according to (6).

It is usually known that the solution for every physically-admissible \( V \) exists, at least, in the equations of mathematical physics. Consequently, the matrix inversion in (7) is well-defined.

We can also invert (7) formally and write
\[ V(T) = (I + TT)^{-1}T . \]

Much less is known about the existence of the inverse in (8). If \( T \) is chosen arbitrarily, it is certainly possible to find such \( T \) that the inverse in (8) does not exist. In DCTMC, \( V \) is updated iteratively by using formula (8). Therefore, existence of the inverse is important. While we do not possess a general proof, numerical simulations for the inverse diffraction problem have encountered no singularities in (8). Of course, the T-matrix used in these iterations is not arbitrary: it is always data-compatible and we can reasonably hope that it approaches the true T-matrix as the iterations progress. We therefore have sufficient empirical evidence that both (7) and (8) are well defined and numerically stable. This does not mean that in some other ISP a singularity can not be encountered. But at least there is reasonable hope that in most practical cases it won’t. We therefore proceed under the assumption that (7) and (8) are numerically stable and establish one-to-one correspondence between the matrices \( T \) and \( V \).

A block diagram of Eq. (6) with all matrix sizes indicated is shown in Fig. 2. Here \( N_s \) and \( N_d \) are the numbers of sources and detectors used (not necessarily equal) and \( N_v \) is the number of volume voxels. For a practical estimate of these numbers, refer to Fig. 1. Let the measurement surfaces \( \Sigma_s \) and \( \Sigma_d \) be identical squares located on the opposite sides of an \( L \times L \times L \) cubic sample as is shown in the Figure. Let the sources and detectors be scanned on an \( L \times L \) square grids and let the sample be discretized on a cubic grid with the same pitch. Then \( N_s = N_d = L^2 \), \( N_v = L^3 \). We can further assume that \( L \gg 1 \). In this case, the following inequalities hold: \( N_s, N_d \ll N_v \ll N_sN_d \).

The first inequality in the above (\( N_s, N_d \ll N_v \)) illustrates Remark 1 in Sec. 2.1 namely that matrices \( A \) and \( B \) are not typically invertible. The second inequality
Solution of the inverse scattering problem by T-matrix completion

Figure 2. Block diagram of Eq. (6) with sizes of all matrices indicated. Here \( N_s \) and \( N_d \) are the numbers of sources and detectors and \( N_v \) is the number of voxels.

\((N_v \ll N_sN_d)\) is important if we want to compare the method developed here to the traditional approaches. For example, in the traditional formulation of the linearized problem, we arrive at the equation \( Kx = \phi \) (see Remark 2 in Sec. 2.1). In this equation, the size of \( K \) is \( N_sN_d \times N_v \). Computing numerically the pseudo-inverse of this matrix is a much more computationally-intensive task than computing the pseudo-inverses of \( A \) and \( B \), which is required by DCTMC. Thus, the relaxation of the strict requirement of diagonality of \( V \) allows one to work with two much smaller “weight matrices” \( A \) and \( B \) instead of one large “weight matrix” \( K \). However, in Sec. 2.4 we explain how the ideas of this paper can be used to accelerate the solution of the linearized problem while enforcing strict diagonality of \( V \).

We denote by \( T_{\text{exp}} \) the “experimental” T-matrix that is compatible with the data (i.e., satisfies (9)) and has the smallest entry-wise norm \( \|T\|_2 \). This matrix is given by

\[
T_{\text{exp}} = A^+\Phi B^+, \tag{9}
\]

where the “+” symbol indicates Moore-Penrose pseudoinverse. Computing \( T_{\text{exp}} \) is the only instance where the method uses the data. Consider the singular value decompositions of \( A \) and \( B \):

\[
A = \sum_{\mu} \sigma^A_{\mu} f^A_{\mu} g^A_{\mu}^* , \quad B = \sum_{\mu} \sigma^B_{\mu} f^B_{\mu} g^B_{\mu}^* , \tag{10}
\]

where star denotes Hermitian conjugation (simultaneous transposition and complex-conjugation). Here \( \sigma^A_{\mu}, f^A_{\mu}, g^A_{\mu} \) is a set of singular values and right and left singular vectors of \( A \), and similarly for \( B \). Using orthogonality of singular vectors, we obtain from (9)

\[
\Psi_{\mu\nu} \equiv \langle f^A_{\mu}, \Phi g^B_{\nu} \rangle = \sigma_{\mu}^A \sigma_{\nu}^B \langle g^A_{\mu}, T f^B_{\nu} \rangle \equiv \sigma_{\mu}^A \sigma_{\nu}^B \tilde{T}_{\mu\nu}. \tag{11}
\]

Here \( \langle x, y \rangle \) denotes the inner product of two vectors, that is, \( \langle x, y \rangle = \sum_{n} x_n^* y_n \). By \( \tilde{T} \) we denote the T-matrix in singular-vector representation while \( T \) that was used previously is the T-matrix in real-space representation. The two representations are related to each other by the transforms

\[
\tilde{T} = R_A^* T R_B , \quad T = R_A \tilde{T} R_B^* , \tag{12}
\]
where \( R_A \) is the orthogonal matrix whose columns are the singular vectors \( g^A_\mu \) while \( R_B \) is the orthogonal matrix whose columns are the singular vectors \( f^B_\mu \).

We now return to Eq. (11) and write its solution as follows:

\[
\tilde{T}_{\mu\nu} = \begin{cases} 
\frac{1}{\sigma^A_\mu \sigma^B_\nu} \Psi_{\mu\nu}, & \text{if } \sigma^A_\mu \sigma^B_\nu > \lambda^2, \\
\text{undetermined}, & \text{if } \sigma^A_\mu \sigma^B_\nu \leq \lambda^2.
\end{cases}
\]

(13)

Here \( \lambda \) is a small regularization parameter. If computations could be performed with infinite precision, we could set \( \lambda = 0 \). In practice, we should take \( \lambda \) to be at least as large as the smallest positive floating-point constant for which a particular implementation of numerical arithmetic adheres to the IEEE standard.

Eq. (13) summarizes our knowledge about the system that is contained in the data. There are few matrix elements of \( \tilde{T} \) that we know with certainty. These can be computed by the first expression in (13). The other matrix elements are in principle unknown. We note right away that the number of known elements of \( T \) can not exceed \( N_s N_d \) but can be, in practice, much smaller. However, even \( N_s N_d \) is a much smaller number than the total number of the matrix elements of \( T \), which is equal to \( N_v \). Using the previously explained estimates, \( N_s N_d / N_v^2 \sim 1/L^2 \). Therefore, only a small fraction of the elements of \( \tilde{T} \) are known. We can collect all such elements into the upper-left block of the matrix, as is schematically illustrated in Fig. 3.

Thus, we can not gain any knowledge about the matrix of \( \tilde{T} \) outside of the shaded area. We can, however, make an initial guess about \( \tilde{T} \), which we denote by \( \tilde{T}_{\text{exp}} \). In this guess, all the unknown elements in the unshaded area of the diagram in Fig. 3 are simply set to zero. To summarize,

\[
(\tilde{T}_{\text{exp}})_{\mu\nu} = \begin{cases} 
\frac{1}{\sigma^A_\mu \sigma^B_\nu} \Psi_{\mu\nu}, & \text{if } \sigma^A_\mu \sigma^B_\nu > \lambda^2, \\
0, & \text{if } \sigma^A_\mu \sigma^B_\nu \leq \lambda^2.
\end{cases}
\]

(14)

This expression is, in fact, equivalent to (9).

Our goal is to fill the unknown elements of \( \tilde{T} \) (the white areas in Fig. 3) in such a way that the corresponding interaction matrix \( V \) (computed according to (8)) is approximately diagonal. This is a general formulation of the problem of matrix completion, expect that the constraint applied to the unknown elements of \( \tilde{T} \) has not been used before, to the best of our knowledge.
Solution of the inverse scattering problem by T-matrix completion

Before proceeding, a few additional remarks need to be made:

**Remark 3: Lack of sparsity of $T_{\text{exp}}$.** The matrix $\tilde{T}_{\text{exp}}$ is sparse because most of its elements are zero. The same is not true for $T_{\text{exp}}$.

**Remark 4: The requirement of data-compatibility.** When we apply the requirement of data-compatibility to the T-matrix in an iterative process, we always do so in singular-vector representation. The requirement means that the elements of $\tilde{T}$ within the shaded block of Fig. 3 must be the same as in $\tilde{T}_{\text{exp}}$; other elements can be arbitrary. Data-compatibility can be enforced iteratively by over-writing the elements in the shaded area with respective elements of $\tilde{T}_{\text{exp}}$.

**Remark 5: Efficient use of data.** The only instance when the data is used in DCTMC is computation of $\tilde{T}_{\text{exp}}$. After this is done, it is sufficient to store in memory only the elements in the shaded block of Fig. 3. In the case of a perfectly well-defined problem, the total number of elements in the data matrix $\Phi$ and in the shaded block are the same, and the effective number of the data points is not changed. In severely ill-posed problems, the former is much larger than the latter. Therefore, computation of $\tilde{T}_{\text{exp}}$ effectively reduces the number of useful data points by eliminating the redundancy of equations. However, none of the actual measurements are discarded in the process which can be very useful in the case when the measurements contain random noise. In the process of computing $\tilde{T}_{\text{exp}}$ from $\Phi$ the random noise is suppressed by averaging. We therefore expect DCTMC to be particularly useful for severely ill-posed problem with strongly over-determined data sets, a typical situation in optical diffusion tomography [4].

**Remark 6: Lack of symmetry of $\tilde{T}$.** Note that $R_{A}^{*} R_{B} \neq \mathbb{I}$. Therefore, $\tilde{T}$ does not possess the same symmetry properties as $T$: $\tilde{T}$ is not necessarily symmetric even if $T$ is. In this respect, the representations considered here differ from the standard representations involving rotations with a single orthogonal matrix $R$, i.e., $R^{*} T R$.

2.3. Defining the iterations

We now define an iterative process in which the matrices $T$ and $V$ are continuously updated so that $T$ is kept data-compatible and $V$ is becoming more diagonally-dominated. The key features of this process are the following:

- $T$ and $V$ are coupled to each other by (7) and (8), which we will use in real-space representation.
- The diagonality of $V$ is “enforced” in real-space representation by either setting all off-diagonal elements of $V$ to zero, or by row-wise summation of all elements to the diagonal, or by some other method.
- Data compatibility of $T$ is "enforced" in singular-vector representation by overwriting the elements of $\tilde{T}$ in the shaded block of Fig. 3 with the respective elements of $\tilde{T}_{\text{exp}}$. The latter is kept in memory and not updated.

- Transformations from real-space to singular-vector representations and back are performed on the T-matrix by rotations (12). Inversion operations (7) and (8) are performed in real-space representation.

- Computational complexity of each iteration is $O(N_v^3)$. Computations are easily parallelizable. $N_v \sim 10^3$ is not problematic even on an inexpensive workstation and $N_v \sim 10^5$ is still feasible but will require a good parallel computational platform. Generally, the method is well-suited for strongly over-determined problems with not extremely large numbers of voxels.

- The problem can be greatly simplified if it is known a priori that the medium can contain a limited number of isolated inhomogeneities (whose location and contrast are unknown. In this case, the limiting factor, is the number of voxels that contain inhomogeneities rather than the total number of voxels.

We can start the iterations from an initial guess for $T$ or for $V$. In the first case, $T_{\text{exp}}$ is used as the initial guess. In the second case, a linearized solution can be used. A fast method to obtain the linearized solution is briefly described in Sec. 2.4.

**Starting iterations from an initial guess for $T$.** Define $\tilde{T}_1 \equiv \tilde{T}_{\text{exp}}$ and starting from $k = 1$ run the following iterations:

(i) Using (12), compute $T_k = R_A \tilde{T}_k R_B^*.$

(ii) Using (8), compute $V_k = V(T_k)$. The latter will, generally, not be diagonal.

(iii) Compute the off-diagonal and diagonal norms of $V_k$. If the ratio of the two is smaller than a predetermined threshold, exit; otherwise, continue to the next step.

(iv) Compute a diagonal matrix $D_k$ by “force-diagonalization” of $V_k$. This operation is denoted by $D_k = \mathcal{D}[V_k]$ and is not equivalent to the usual operation of diagonalization. There are several heuristic definitions of $\mathcal{D}[V]$ such as setting all the off-diagonal elements of $V$ to zero or column-wise or row-wise summation to the diagonal, etc.

(v) Optionally, if using additional constraints, apply these to $D_k$. For example, a physical constraint may require that all elements of $D_k$ be non-negative. The operation is denoted by $D_k' = \mathcal{C}[D_k]$.

(vi) Optionally, apply the “roughening” operation to $D_k'$. The diagonal elements of $D_k'$ that are smaller in norm than a certain predetermined threshold can be deemed as insignificant and set to zero. This will greatly increase the computational efficiency of the next step. The operation is denoted by $D_k'' = \mathcal{R}[D_k']$.

(vii) Using (7), compute $T_k' = T(D_k'')$ in real-space representation.

(viii) Using (12), compute $\tilde{T}_k' = R_A^* T_k'R_B$ (rotate to singular-vector representation).
(ix) Overwrite the elements of $\tilde{T}'_k$ in the shaded block of Fig. 3 with the nonzero elements of $\tilde{T}_{\exp}$. This will create a data-compatible T-matrix in singular-vector representation. The corresponding operation is $\tilde{T}_{k+1} = \mathcal{C}[\tilde{T}_k']$.

(x) Advance the iteration index $k \to k + 1$ and go to Step (i).

Starting from an initial guess for $V$. This is a minor variation of the method. Let’s assume that an initial guess $V_g$ is available, e.g., from solution of the linearized problem. Let’s assume that $V_g$ is strictly diagonal. Then define $D_1 = V_g$, set $k = 1$ and go to Step (v) of the above algorithm. In this case $T_1$ is not defined and the first obtained approximation to the T-matrix is $T_2$.

2.4. Fast computation of linearized inverses

As an aside, consider a couple of fast methods for solving the linearized ISP. The result can be used as the initial guess for the above iterative algorithm. Although in this Subsection we will assume that $V$ is strictly diagonal, and enforce this condition rigorously, the methods grow from the general theoretical framework described elsewhere in this paper for a more general $V$. While these methods are fairly obvious and simple in application, we are not aware of any instances when they have been actually used (except for the symmetry-based methods for optical diffusion tomography [22–24], where a similar acceleration is obtained by exploiting translational symmetry of the background medium and the grids of sources and detectors). This is most likely so because the rearrangement of the product $A_{nl}B_{lm}$ into a single matrix $K_{p(n,m),l}$ (as described in Remark 2) tends to obscure the basic algebraic structure of the equations. Here we describe methods that do not depend on symmetry and are applicable in arbitrary imaging geometry.

Method 1. Consider the linearized equation

$$\sum_l A_{nl}x_l B_{lm} = \Phi_{nm} ,$$

which is obtained from (6) by making the first Born approximation and assuming that $V$ has the numbers $x_l$ on the diagonal and zeroes elsewhere. We now use (10) for $A_{nl}$ and $B_{lm}$. A straightforward calculation results in:

$$\sigma^A_{\mu} \sigma^B_{\nu} \sum_l (g^A_{\mu})_l x_l (f^B_{\nu})_l = \Psi_{\mu\nu} ,$$

where $\Psi_{\mu\nu}$ is defined by the first identity in (11). We then can write

$$\sum_l (g^A_{\mu})_l x_l (f^B_{\nu})_l = \begin{cases} \frac{1}{\sigma^A_{\mu} \sigma^B_{\nu}} \Psi_{\mu\nu}, & \text{if } \sigma^A_{\mu} \sigma^B_{\nu} > \lambda^2 , \\ \text{undetermined}, & \text{if } \sigma^A_{\mu} \sigma^B_{\nu} \leq \lambda^2 . \end{cases}$$
The above defines $M$ linear equations with respect to $N_v$ unknowns $x_l$, where $M$ is the number of pairs $(\sigma^A_\mu, \sigma^B_\nu)$ that satisfy the condition $\sigma^A_\mu \sigma^B_\nu > \lambda^2$. In a severely ill-posed problem, this number is expected to be much smaller than the total number of data points, $N_s N_d$. Thus, we have achieved data reduction: namely, we have reduced a very large data set contained in the matrix $\Phi$ to a much smaller set containing only $M$ data points. Now, the singular vectors $g^A_\mu$ and $f^B_\nu$ and the corresponding singular values are easy to compute because matrices $A$ and $B$ are comparatively small. We can, therefore, arrange all the equations contained in the first case of (17) into a linear set \[
abla \sum_l C^{\mu \nu, l} x_l = b^{\mu \nu}, \]
where $C^{\mu \nu, l} = (g^A_\mu)^l (f^B_\nu)^l$ and $b^{\mu \nu} = (\sigma^A_\mu \sigma^B_\nu)^{-1} \Psi_{\mu \nu}$, and only such pairs of indexes $(\mu, \nu)$ are used that the first condition in (17) holds. The obtained set of linear equations is much smaller than the original set (15) and can be easily solved by regularized Tikhonov pseudo-inverse.

Method 2. This method is also based on separability of $K_{p(n,m),l}$, but it does not achieve the optimal data reduction; it simply makes use of the separability for purely numerical purposes. Assume that we wish to solve the equation $K x = \phi$ where $\phi$ and $x$ are vectors unrolled from the respective matrices as described in Remark 2. Also assume that the problem is strongly overdetermined and that we wish to solve it by computing the pseudoinverse of $K$. One approach is simply to discard the majority of equations as redundant. But this does not help with the random measurement noise averaging. Instead, we wish to utilize all available measurements. Then one possible approach to computing the pseudoinverse is to compute $K^* K$ and $x^+ = (K^* K)^{-1} K^* \phi$, where "reg" indicates Tikhonov regularization. It turns out that the most time consuming operation in the above is the computation of $K^* K$. The inversion can be performed by (i) regularization $K^* K \rightarrow K^* K + \lambda^2 I$ and then (ii) solving the resulting set by conjugate-gradient descent, with the computational complexity of $O(N^2_v N_{\text{iter}})$ ($N_{\text{iter}}$ - number of conjugate-gradient iterations). This is not problematic up to $N_v \sim 10^5$. But the direct computation of the product $K^* K$ has the complexity of $N^2_v N_s N_d$, which is much larger than that of the former operation. If nothing is known about $K$, complexity of the matrix-matrix multiplication can not be reduced. But the separability of $K$ is a useful fact. Indeed, we can write $K_{nm,l} = A_{nl} B_{lm}$ and
\[
(K^* K)_{kl} = \sum_{nm} K^*_{nm,l} K_{nm,k} = \sum_n (A^*_{nl} A_{nk}) \sum_m (B^*_{lm} B_{km}). \tag{18}
\]
Thus the double summation over $n$ and $m$ has factored into two single summations. Now the complexity of computing $K^* K$ is reduced to $O(N^2_v \max(N, N_d))$, which is comparable to that of computing the pseudoinverse of $K^* K$.

2.5. Fast rotations

One computational aspect that needs additional discussion is the efficiency of rotations required by the steps (viii), (ix) and (i) of the iterative scheme described in Sec. 2.3. More specifically, these rotations require taking the T-matrix in the real-space representation,
rotating it to the singular-vector representation, overwriting the matrix elements in the shaded block of Fig. 3 with the nonzero elements of $\tilde{T}_{\text{exp}}$ and, finally, rotating the result back to the real-space representation. These operations can be written as

\begin{align}
(viii) : & \quad T \rightarrow \tilde{T} = R_A^T R_b, \\
(ix) : & \quad \tilde{T} \rightarrow \tilde{T}' = \tilde{T} - \tilde{\Delta} + \tilde{T}_{\text{exp}}, \\
(i) : & \quad \tilde{T}' \rightarrow T' = R_A \tilde{T}' R_b^*. 
\end{align}

Here $\tilde{\Delta}$ is a matrix that coincides with $\tilde{T}$ in the shaded block and is zero everywhere else. Combining all operations in (19) in one, accounting for the sparsity of $\tilde{\Delta}$ and for the invertibility of rotations, we arrive at the result that the three operations defined above can be written as

$$T \rightarrow T + T_{\text{exp}} - P_A T P_B^*,$$

where $P_A$ is the projection operator defined by $P_A = M^*[R_A]M[R_A]$. Here $M[R]$ is the mask operator. It takes the square matrix $R$ and eliminates all lines in this matrix except for the first $M$ lines, where $M$ is the number of columns in the shaded block. $M^*$ is a similar column-wise operation. It can be seen that the computation of the term $P_A T P_B^*$ can be performed efficiently by writing

$$P_A T P_B^* = M^*[R_A]\left\{M[R_A]T M^*[R_B]\right\}M[R_B].$$

Now, since the matrix $M[R_A]$ contains much fewer entries than $R_A$, the product in the curly brackets can be computed very fast. After that the outer-layer product is computed in a similar manner. On the other hand, $T_{\text{exp}}$ is computed once and stored in memory. Consequently, the rotations of $T$ can be performed in a computationally-efficient manner and do not restrict the method performance.

3. An example of discretization: scalar wave equation

Consider scalar field $u(\mathbf{r})$ (e.g., pressure wave in ultrasound imaging) and the wave equation

$$\left[\nabla^2 + k_0^2 \epsilon(\mathbf{r})\right] = -4\pi S(\mathbf{r}),$$

where $\epsilon(\mathbf{r}) = 1$ outside of the bounded domain $\Omega$ (the sample) and the factor $-4\pi$ has been introduced for convenience. We can re-write this in the form

$$\left[\nabla^2 + k_0^2 \right] u(\mathbf{r}) = -4\pi [\eta(\mathbf{r}) + S(\mathbf{r})], \quad \eta(\mathbf{r}) = k_0^2 \frac{\epsilon(\mathbf{r}) - 1}{4\pi}.$$

The field $u$ satisfies Lippman-Schwinder equation

$$u(\mathbf{r}) = u_0(\mathbf{r}) + \int G_0(\mathbf{r}, \mathbf{r}')\eta(\mathbf{r}')u(\mathbf{r}')d^3r',$$

where $u_0(\mathbf{r}) = \int G_0(\mathbf{r}, \mathbf{r}')S(\mathbf{r}')d^3r'$ is the incident field and

$$G_0(\mathbf{r}, \mathbf{r}') = \frac{\exp(i k_0|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|}.$$
is the unperturbed Green’s function, which satisfies
\[
[\nabla^2 + k_0^2] G_0(r, r') = -4\pi \delta(r, r') .
\] (26)

We now proceed with discretization. Let the sample be discretized into cubic voxels \( C_k \) of volume \( h^3 \) each. We make the following approximations:
\[
\eta(r) = \eta_k = k_0^2(\varepsilon_k - 1)/4\pi
\]
and
\[
u(r) = u_k, \quad u_0(r) = u_{0k} \quad \text{for} \quad r \in C_k.\]
We then re-write (24) as
\[
u_k = u_{0k} + \sum_l \eta_l u_l \int_{r' \in C_l} G_0(r, r') d^3 r', \quad r \in C_k .
\] (27)

To approximate the above integral, we must consider the two cases \( l = k \) and \( l \neq k \) separately. For \( l \neq k \) the standard approximation is
\[
\int_{r' \in C_l} G_0(r, r') d^3 r' \approx h^3 G_0(r_k, r_l) \equiv h^3 \Gamma_{kl} , \quad r \in C_k \neq C_l ,
\] (28)
where \( r_k \) is the center of \( C_k \). For \( l = k \), a more careful evaluation of the integral is required because the integrand contains a singularity in this case. It is a standard approximation to assume that \( k_0 h \ll 1 \) so that the exponent in the expression for \( G_0 \) can be approximated by unity. We then place \( r \) in the center of \( C_k \) and obtain the integral
\[
\int_{r' \in C_k} G_0(r_k, r') d^3 r' = \int_{-h/2}^{h/2} dx \int_{-h/2}^{h/2} dy \int_{-h/2}^{h/2} dz \frac{1}{\sqrt{x^2 + y^2 + z^2}} = \xi h^2 .
\] (29)

Here \( \xi = \log(26 + 15\sqrt{3}) - \pi/2 \approx 2.38 \). An alternative estimate is obtained if we replace integration over the cubic voxel by integration over a ball of equivalent volume, which results in a much simpler integration and \( \xi = (9\pi/2)^{1/3} \approx 2.42 \) (fairly close to the former result). The two approaches to integration can be applicable in different physical situations. For example, integration over a ball may be more appropriate if we wish to describe scattering by a collection of spherical inclusions rather than voxelization of a medium on a cubic grid. In both cases, there is an approximation involved because we have placed the vector \( r \) in the center of the voxel.

We can now use the approximations for the integral to re-write (27) as a set of linear algebraic equations:
\[
u_k = \frac{1}{1 - \xi h^2 \eta_k} \left( u_{0k} + h^3 \sum_{l \neq k} \Gamma_{kl} \eta_l u_l \right) .
\] (30)

Further, it is convenient to introduce the moments \( d_k = h^3 \eta_k u_k \). In the case of electromagnetic scattering, these quantities would represent the dipole moments of voxels, but for the case of scalar waves, it is more appropriate to speak about the monopole moments (not to be confused with Dirac monopoles). In terms of \( d_k \), the system takes an especially simple form, namely,
\[
d_k = \alpha_k \left( u_{0k} + \sum_{l \neq k} \Gamma_{kl} d_l \right) , \quad \alpha_k \equiv \frac{h^3 \eta_k}{1 - \xi h^2 \eta_k} .
\] (31)
We can refer to the quantity $\alpha_k$ defined above as to the “susceptibility” of $k$-th voxel. We emphasize that discretization is a valid procedure as long as the term $\xi h^2 \eta_k$ in the denominator of $\alpha_k$ is small compared to unity. However, for better precision of discretization, this correction to $\alpha_k$ should not be disregarded.

The inverse problem can now be formulated in terms of $\alpha_k$'s. Indeed, let the interaction operator $V$ contain $\alpha_k$'s on the diagonal and zeroes everywhere else. Then we can write in matrix notations $d = V(u_0 + \Gamma d)$, where $d$ and $u_0$ are vectors of length $N_v$. From the formal solution $d = (I - V \Gamma)^{-1} V u_0$ and comparing to (7), we find that $d = T u_0$. Further, at the detection plane, the fields scattered by the sample is given by $u_s(r_d) = \int G_0(r_d, r) \eta(r) u(r) d^3r$, $r_d \in \Sigma_d$, which, upon similar discretization, transforms to $u_s = Ad$. Similarly, $u_0 = BS$. We therefore arrive again at the inverse problem (6),(7) in which $\Gamma$ is determined by (28) and $A$ and $B$ are determined by sampling of $G_0(r, r')$ (in this case, singularity of $G_0$ is not encountered).

Therefore, we can pose the following problem: given a set $\Phi$ of measurements of $u_s$, find the interaction matrix $V$ that is as diagonal as possible. Once this is done, the diagonal elements of $V$ contain the quantities $\alpha_k$. If $\xi$ and $\alpha_k$ are known, we can easily compute $\eta_k = \alpha_k/h^2(h + \xi \alpha_k)$.

4. A toy problem

Consider Eq. (31) for the case of just two voxels or two discrete small scatterers of strengths $\alpha_1$ and $\alpha_2$. Assume that we wish to reconstruct these quantities from scattering measurements involving one source $S$ and two detectors $D_1$ and $D_2$, as is schematically illustrated in Fig. 4. The size of the data set is in this case $N_s N_d = 2$, so that the problem is perfectly determined. Also, $\Gamma_{12} = \Gamma_{21} = g$, $\Gamma_{11} = \Gamma_{22} = 0$.

The set (31) consists in this simple case of two equations

\[ d_1 = \alpha_1 (u_0 + gd_2), \quad d_2 = \alpha_2 (u_0 + gd_1), \]

where $u_0$ is the incident field created by the source at the locations of the scatterers (in the case considered, $u_{10} = u_{20} = u_0$) and the detectors measure the linear combinations $\Phi_1 = (B_1 d_1 + B_2 d_2)/u_0$ (the first detector) and $\Phi_2 = (B_1 d_2 + B_2 d_1)/u_0$ (the second detector). The problem is to use the measurements of $\Phi_1$ and $\Phi_2$ to find $\alpha_1$ and $\alpha_2$. After some manipulation, we can write the nonlinear equations coupling $(\alpha_1, \alpha_2)$ to...
Figure 5. Left: Illustration of the region of convergence of the inverse Born series defined by the inequalities in (36). Axes of the plot are $x_1$ and $x_2$. Both conditions are satisfied in the dark blue region, only one in light blue region. Inverse Born series diverge outside of the dark blue region. The plot illustrates convergence of the series only for purely real $\alpha_k$'s. Right: Relative error $E$ (37) after four iterations of DCTMC for the toy problem. Same axes as in the left panel are used.

(\Phi_1, \Phi_2) as

\[
(1 - g^2 \alpha_1 \alpha_2) \Phi_1 = \alpha_1(1 + g \alpha_2) + \beta \alpha_2(1 + g \alpha_1), \quad (1 - g^2 \alpha_1 \alpha_2) \Phi_2 = \alpha_2(1 + g \alpha_1) + \beta \alpha_1(1 + g \alpha_2),
\]

where $\beta = B_2 / B_1$. These equations have a unique solution if $\beta^2 \neq 1$:

\[
\alpha_1 = \frac{\beta \Phi_2 - \Phi_1}{\beta^2 - 1 + g(\beta \Phi_1 - \Phi_2)}, \quad \alpha_2 = \frac{\beta \Phi_1 - \Phi_2}{\beta^2 - 1 + g(\beta \Phi_2 - \Phi_1)}.
\]

(33)

If $\beta^2 = 1$, application of (33) to perfect data results in a 0/0-type uncertainty while application to noisy data can result in spurious solutions $\alpha_1 = \alpha_2 = \pm g$. We therefore assume that $\beta^2 \neq 1$. Then the reconstructions depend on the data continuously except for the lines $\beta \Phi_1 - \Phi_2 = (1 - \beta^2)/g$ and $\beta \Phi_2 - \Phi_2 = (1 - \beta^2)/g$, where the inversion formulas are singular.

Let us find the condition under which a series expansion of the inverse solution (34) in powers of $\Phi_1$ and $\Phi_2$ converges. This is the condition of convergence of the inverse Born series [9,19,20]. We note that, for a more general ISP, a sufficient condition of convergence of inverse Born series was obtained [19]. For the toy problem discussed here, we can obtain a sufficient and necessary condition of convergence, which is

\[
\left| \frac{g}{\beta^2 - 1}(\beta \Phi_1 - \Phi_2) \right| < 1 \quad \text{AND} \quad \left| \frac{g}{\beta^2 - 1}(\beta \Phi_2 - \Phi_1) \right| < 1
\]

(35)

We can express this condition in terms of the model values of $\alpha_1, \alpha_2$ by using (33). Let $x_k = g \alpha_k^{mod}$, where “mod” refers to the the model values of $\alpha_k$. Then the convergence
Solution of the inverse scattering problem by T-matrix completion

condition reads
\[
\left| \frac{x_2(1 + x_1)}{1 - x_1 x_2} \right| < 1 \quad \text{AND} \quad \left| \frac{x_1(1 + x_2)}{1 - x_1 x_2} \right| < 1.
\] (36)

The solution to these two inequalities is illustrated in Fig. 5 (left panel).

We can now compare this convergence result for the inverse Born series to a similar result for DCTMC. For the toy problem considered, DCTMC can be run analytically for a few iterations, and these results can be used to prove a sufficient condition for convergence of the iterations. This condition is \(|x_1| < 1\) AND \(|x_2| < 1\). This defines a square region between the lines \(x_1 = \pm 1\) and \(x_2 = \pm 1\), which partially overlaps with the region of convergence shown in Fig. 5 (left panel). In practice, we have observed that DCTMC converges in a much wider area than the one defined by the above sufficient condition. In particular, the method appears to converge for most positive values \(x_1\) and \(x_2\) in just a few iterations. This is illustrated in Fig. 5 (right panel), where we plot the relative error

\[
E = \sqrt{\left| \frac{\alpha_1^{\text{rec}}}{\alpha_1^{\text{mod}}} - 1 \right|^2 + \left| \frac{\alpha_2^{\text{rec}}}{\alpha_2^{\text{mod}}} - 1 \right|^2}.
\] (37)

Here “rec” and “mod” refer to reconstruction and model.

5. Numerical simulations

Our numerical results concern the inverse problem defined in Sec. 3 and the same mathematical formalism will be used. We have implemented reconstruction of the quantities \(\alpha_k\) in a cubic sample discretized into an \(L \times L \times L\) grid with the pitch \(h\). The measurement planes with sources and detectors placed on an \(L \times L\) square grid with the same pitch \(h\) were located at varying distance \(H\) from the sample surface. The wavelength \(\lambda = 2\pi/k_0\) also varied; the relevant dimensionless parameter is \(k_0 h\).

In all cases, the sample was a cube with \(\alpha_k = \alpha_0\) in all voxels except for the 8 voxels in the center, where we have used \(\alpha_k = 2\alpha_0\). The value of \(\alpha_0\) was allowed to vary, and the characteristic dimensionless parameter is \(\alpha_0/h\). We will refer to these values as to the model. We emphasize that the reconstructions did not utilize any a priori knowledge of \(\alpha_k\)’s and that the problem of determination \(\alpha_k\)’s is strongly nonlinear even if all \(\alpha_k\)’s are the same in the model.

We start by considering inversion errors in the case \(L = 6\) \((N_v = 216\) voxels\), \(k_0 h = 1\) and \(H = h\). Note that \(k_0 h = 1\) is the relatively short-wavelength regime in which the discretization of Sec. 3 is, strictly speaking, invalid. However, we can consider (31) as the first-principle equation, without regard to the underlying physical model. The reason we have made this choice is because the ill-posedness of the ISP related to the diffraction resolution limit is suppressed in the short-wavelength regime, while the nonlinearity is, on the contrary, strong. Thus, we can investigate the case wherein the reconstruction is difficult due to the nonlinearity alone rather than due to both nonlinearity and ill-posedness. In Fig. 6 we compare the root-mean-square error (RMSE) \(\chi\) of the reconstructed values of \(\alpha_k/h\), for a linearized reconstruction (based
Figure 6. RMSE $\chi$ vs dimensionless parameter $\alpha_0/h$ for a linearized reconstruction (Lin) and for the nonlinear method described here (Nonlin). Points well below the green line marked “Thresh” represent an acceptable level of error.

on computing the pseudo-inverse of $K$) and for the nonlinear method described here. RMSE is defined by

$$\chi = \left[ \frac{1}{N_v} \sum_{k=1}^{N_v} \left( \frac{\alpha_{k}^{\text{rec}}}{h} - \frac{\alpha_{k}^{\text{mod}}}{h} \right)^2 \right]^{1/2},$$

where “rec” and “mod” refer to “reconstruction” and “model”. In the nonlinear reconstruction, the iterations were stopped when the convergence became relatively slow (see typical convergence plots in Fig. 7). It can be seen that the nonlinear reconstruction gives much better precision than the linear one. Note that $\alpha_k/h = h^2\eta_k/(1 - \xi h^2\eta_k)$. As was explained above, the discretization is valid as long as $\xi h^2\eta_k \ll 1$; otherwise, smaller values of $h$ must be used. Therefore, the contrast $\alpha_0/h = 2 \times 0.12 = 0.24$ (in the central voxels), is close to the limit of applicability of the underlying theory. Also, taking into account that $k_0h = 1$ and using $\xi = 2.38$, we find that the model assumes $\epsilon_k = 2.17$ in the outlying voxels and $\epsilon_k = 2.92$ in the central voxels – a reasonably high contrast compared to the surrounding medium (where $\epsilon = 1$), which leads to a strong nonlinearity of the ISP.

We next look at convergence. In Fig. 7, we plot $\chi$ as a function of the iteration number $k$ for different distances between the measurement planes and the sample, $H$ (left panel) and for different values of $k_0h$ (right panel). As can be seen, the initial fast convergence crosses over to a much slower decay around $k = 200$. Similar behavior with fast initial convergence and then a very slow decay has been observed in many examples with varying values of $\alpha_0/h$ and other parameters. Usually the cross-over takes place when $\chi$ is already reasonably small so that the iterations can, in principle, stop. This cross-over to slow convergence is a characteristic feature of many iterative schemes. However, there exists a reasonable hope that the speed of convergence can be improved by changing the prescription of one of the heuristic operations such as the “force-diagonalization” $D[V]$ (Step (iv) of the iterative algorithm of Sec. 2.3), application of physical constraints, “roughening” (Step (vi)), etc. At this point, we note the counter-
intuitive fact that the speed of convergence is improved with $H$. Of course, we do not expect this tendency to hold for arbitrarily large $H$; in fact, for the problem at hand, the optimal $H$ is close to $6h$. This fact underscores the importance of looking at the sample from the “right” distance.

In the right panel of Fig. 7, we illustrate the influence of the wavelength on convergence. The parameter $k_0h$ is varied from 0.1 to 8.0, the last value being fairly unrealistic from the point of view of medium discretization. However, our goal at the moment is to invert (31) without regard to the underlying physical model, and in (31) $k_0h$ can be arbitrary. It can be seen that the convergence is indeed improved in the short-wavelength regime. At $k_0h = 8.0$, the slow convergence regime is all but eliminated. This result is interesting in itself and will require detailed research to gain a better understanding of the reasons for and the ways to overcome the slow convergence.

6. Conclusion

This paper contains an mathematical formulation and initial numerical validation of a novel method for solving nonlinear inverse scattering problems. The method is based on an iterative completion of the unknown entries of the T-matrix and we refer to it as the data-consistent T-matrix completion (DCTMC) The most promising result is that the method solves the problem in principle, including the cases when the nonlinearity is very strong and many other iterative methods are expected to fail. However, many additional tests and a detailed study of convergence are required to fully understand the advantages and drawbacks of the proposed method.
Solution of the inverse scattering problem by T-matrix completion

Acknowledgments

This research was supported in part by US NSF under Grant DMS 1115616. The authors are grateful to J.C. Schotland for very useful discussions.

References

[1] Snieder R 1998 *Inverse Problems* **14** 387404
[2] Seo J K and Woo E J 2012 *Nonlinear Inverse Problems in Imaging* (Wiley)
[3] Boas D A, Brooks D H, Miller E L, DiMarzio C A, Kilmer M, Gaudette R J and Zhang Q 2001 *IEEE Signal Proc. Mag.* **18**(6) 57–75
[4] Arridge S R and Schotland J C 2009 *Inverse Problems* **25** 123010
[5] Bronstein M M, Bronstein A M, Zibulevski M and Azhari H 2002 *IEEE Trans. Med. Imag.* **21** 1395–1401
[6] Devaney A J 1984 *IEEE Trans. Geosci. Remote Sensing* **GE-22** 3–13
[7] Berryman J G and Kohn R V 1990 *Phys. Rev. Lett.* **65**(3) 325–328
[8] Isaacsosn D, Mueller J L, Newell J C and Siltanen S 2004 *IEEE Trans. Med. Imag.* **23** 821–828
[9] Arridge A, Moscow S and Schotland J C 2012 *Inverse Problems* **28** 035003
[10] Carney P S, Frazin R A, Bozhevolnyi S I, Volkov V S, Boltasseva A and Schotland J C 2004 *Phys. Rev. Lett.* **92** 163903
[11] Belkebir K, Chaumet P C and Sentenac A 2005 *J. Opt. Soc. Am. A* **22** 1889–1897
[12] Bao G and Li P 2007 *Opt. Lett.* **32** 1465–1467
[13] Newton R G 1966 *Scattering theory of waves and particles* (New York: McGrow-Hill)
[14] Colton D and Kress R 1998 *Inverse Acoustic and Electromagnetic Scattering Theory* vol 93 of *Applied Mathematical Scieinces* (Berlin: Springer)
[15] Tarantola A 2005 *Inverse Problem Theory* (Philadelphia: SIAM)
[16] Aster R C, Borchers B and Thurber C H 2005 *Parameter Estimation and Inverse Problems* (Amsterdam: Elsevier)
[17] Engl H W and Kugler P 2005 *Multidisciplinary Methods for Analysis Optimization and Control of Complex Systems Mathematics in Industry* vol 6 (Springer) chap Nonlinear inverse problems: Theoretical aspects and some industrial applications, pp 3–47
[18] Markel V A, O’Sullivan J A and Schotland J C 2003 *J. Opt. Soc. Am. A* **20**(5) 903–912
[19] Moskow S and Schotland J 2008 *Inverse Problems* **24** 065005
[20] Moskow M and Schotland J 2009 *Inverse Problems* **25** 095007
[21] Watzenig D 2007 *ei Elektrotechnik und Informationstechnik* vol 124 (Springer) chap Bayesian inference for inverse problems - statistical inversion, pp 240–247
[22] Markel V A and Schotland J C 2004 *Phys. Rev. E* **70**(5) 056616
[23] Schotland J C 1997 *J. Opt. Soc. Am. A* **14**(1) 275–279
[24] Markel V A and Schotland J C 2002 *J. Opt. Soc. Am. A* **19**(2) 558–566