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A direct method for the inversion of physical systems

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Abstract. A general algorithm for the direct inversion of data to yield unknown functions entering physical systems is presented. Of particular interest are linear and non-linear dynamical systems. The potential broad applicability of this method is examined in the context of a number of coefficient-recovery problems for partial differential equations. Stability issues are addressed and a stabilization approach, based on inverse asymptotic tracking, is proposed. Numerical examples for a simple illustration are presented, demonstrating the effectiveness of the algorithm.

1. Introduction

Consider a physical system governed by an operator equation of the form

$$A\big(V, u(V)\big) = 0 \tag{1}$$

where, for each choice of the function V, (1) is uniquely solvable for u, the *forward solution*. The notation $u(V)$ is used to indicate that u depends on V. Of particular interest are systems governed by evolution-type equations, such as

$$\begin{aligned} &\frac{\partial u}{\partial t} = T\big(V, u(V)\big) \qquad && t > 0 \\ &u = u_0 && t = 0. \end{aligned} \tag{1'}$$

The inverse problem of interest is to determine the function V by data measurements $d = \{d_j\}$, which are related to V through equations of the form

$$L(u_j, V) = f_j(d_j, u_j) \qquad j = 1, 2, \ldots \tag{2}$$

where each $L(u_j, V)$ is an operator, possibly non-linear, acting on u_j and V. We shall assume here that L is a linear operator in V. In the context of evolution systems such as (1'), each d_j may represent a data signal as a function of time. The solution method proposed in the present paper involves inverting the *coupled* equations (1) and (2) to determine V from d. The key point is that these equations may be formally decoupled to yield a useful algorithm for inversion.

In practice, one typically solves an inverse problem of the type (1), (2) by using a least-squares minimization criterion (see, e.g. [1] and the references therein). The present

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method significantly differs in this regard in that the inversion is *direct*, eliminating the need for computationally expensive iterative searching procedures.

The development of the present method was motivated by the important quantum dynamics problem of determining potential energy surfaces from laboratory data. There have been a number of algorithms which seek to invert time-independent data (e.g. scattering and spectral data, etc). With the emergence of new ultrafast pump–probe laser techniques, laboratory data measurements can be performed on the time scales of the dynamical events themselves [11]. The proposed algorithm has been designed to take advantage of these new developments, although it may also be adapted to treat time-independent measurements. Some precedent for this approach exists in a recently proposed inverse scattering algorithm [12]. A direct procedure of limited applicability for the inversion of temporal data has been proposed by Bernstein and Zewail [2] and Gruebele *et al* [7]. In addition, this latter approach does not lend itself to use in inverse problems from other disciplines. The application of the present algorithm to the problem of potential surface determination is introduced in section 3 of this work, and will be explored more fully elsewhere.

The primary goal of the present paper is to establish a first step in an alternative means for the inversion of physical systems. This is accomplished by presenting a new general algorithm for direct inversion, and illustrating its use, including a proposed stabilization method, through a simple example. The character of this work is formal, and certain mathematical issues, such as characterizing admissible data, are not addressed.

This paper is organized as follows. The inversion algorithm is presented in section 2. In section 3 the logic of the algorithm is considered for representative inverse problems from the areas of heat conduction, population dynamics and quantum-mechanical systems. The latter example is explored in more detail in section 4, where a stabilization scheme is proposed. The paper concludes with numerical examples, testing the effectiveness of the inversion scheme in a simple quantum mechanical illustration, in section 5.

2. The algorithm

The proposed algorithm consists of three steps:

(i) Formally invert the system (2) to express the unknown V in terms of the data d and the (unknown) forward solution u

$$V = \mathcal{V}[d, u]. \tag{3}$$

(ii) Input (3) into equation (1) and solve the resulting system for u.

(iii) The solution u obtained in step (ii) is substituted into the right-hand side of expression (3), thus determining V *explicitly* in terms of the data d.

The existence of the inverse for the available values of u in (3) is tantamount to assuming that the data is complete. Regions of singularity of (3) thus indicate those parts of V that cannot be determined by the particular set of data. In practice a regularized form of (3) would probably be employed to deal with the latter situation when it arises. Assuming that the solution in (3) exists, then the steps (i)–(iii) are strictly identities, and thus provide a rigorous foundation for the algorithm. The key issues are the introduction of stabilization and regularization in the presence of incomplete and noisy data. A full exploration of these matters is beyond the scope of the present work, but some examination of these points will be made.

Step (i) of this algorithm begins by expanding the unknown V as

$$V = \sum_p a_p \phi_p \tag{4}$$

where the set $\{\phi_p\}$ forms a basis in the space in which V is presumed to lie. The basis $\{\phi_p\}$ might have either global or local support. The coefficients $\{a_p\}$ are to be determined. Substitution of (4) into equation (2) yields the system of equations

$$\sum_p a_p L_j \phi_p = f_j(d_j, u_j) \qquad j = 1, 2, \ldots$$

which can be written more compactly as

$$M \cdot a = f \tag{5}$$

where a is the vector of coefficients a_p, and

$$(M)_{jp} = L_j \phi_p \qquad \forall j, p.$$

If the linear operator M is invertible in some suitable sense, then (5) and (4) yield the expression

$$V = \sum_p (M^{-1} \cdot f)_p \phi_p \equiv \mathcal{V}[d, u] \tag{6}$$

corresponding to (3). Substituting (6) into (1) and solving the resulting (highly non-linear) equation will yield u and complete step (ii). Finally, this u will be substituted into the right-hand side of (6) to determine the desired V. In the case of an evolution system of the form (1′), one can in principle perform step (ii) by direct time integration of the non-linear system, thus avoiding computationally expensive iterative schemes.

Remark 1. As mentioned above, it is important to recognize that the data d may contain only partial information concerning the function V. Erroneous conclusions can arise by attempting to invert such a data set onto the entire V. This type of occurrence will manifest itself in the existence of a non-trivial nullspace for the linear operator M of equation (5). Procedures for determining the particular solution a of (5) to be used in the subsequent inversion steps should have their own built-in safeguards, based on properties of the underlying physical system (e.g. smoothness of V), regarding the extraction of erroneous results from the data.

3. Examples

In order to illustrate the potential broad applicability of these ideas, the present method is used to reformulate inverse problems from three distinct fields. Only the last of the examples will be numerically explored here.

3.1. Heat conduction

Consider the inverse problem of determining the unknown source function $V = V(x)$ in the parabolic boundary value problem

$$u_t(x,t) = u_{xx}(x,t) + V(x)u(x,t) \qquad 0 < x < L,\ t > 0 \tag{7a}$$

$$u(x,0) = u_0(x) \qquad 0 < x < L \tag{7b}$$

$$u(0,t) = h_0(t) \qquad t > 0 \tag{7c}$$

$$u(L,t) = h_L(t) \qquad t > 0 \tag{7d}$$

from the data

$$u(x,t^*) = d(x) \qquad 0 < x < L \tag{7e}$$

where $t^* > 0$ is a fixed point in time.

A relation of the form (2) can be obtained by setting $t = t^*$ in the differential equation (7*a*)

$$u_t(x,t^*) = u_{xx}(x,t^*) + V(x)u(x,t^*)$$

or, in light of (7*b*) and (7*e*)

$$V(x)d(x) = u_t(x,t^*) - d''(x).$$

If $d(x)$ is never zero, then q can be written as

$$V(x) = \frac{u_t(x,t^*;V) - d''(x)}{d(x)}$$

$$\equiv \mathcal{V}[d,u]. \tag{8}$$

Note that there is no need for the basis expansion (4) in this problem. This leads to the auxiliary boundary value problem

$$\begin{aligned} &u_t(x,t) = u_{xx}(x,t) + \mathcal{V}[d,u]u(x,t) && t > 0,\ 0 < x < L \\ &u(x,0) = u_0(x) && 0 < x < L \\ &u(0,t) = h_0(t) && t > 0 \\ &u(L,t) = h_L(t) && t > 0 \end{aligned} \tag{9}$$

which is to be solved for u. The function V is then obtained from (8). The reformulated problem (9), a special case of the present method, is an example of what is known as a trace-type functional problem [3].

3.2. Age-structured population dynamics

Let $\rho(a, t)$ represent the population density of a species as a function of age a and time t. One possible model for the dynamics of this population is known as the *Lotka–von Foerster* model [13]

$$\begin{aligned} &\rho_t(a,t) + \rho_a(a,t) + V(a)\rho(a,t) = F(a,t,\rho) && 0 < a < L,\ t > 0 \\ &\rho(a,0) = \rho_0(a) && 0 < a < L \\ &\rho(0,t) = h(t) && t > 0 \end{aligned} \tag{10}$$

where L is an upper bound on the maximum lifespan of the species, and F is a source term reflecting births, migration, harvesting, etc. Consider the inverse problem of determining the death rate V in this first-order hyperbolic equation from a knowledge of the total populations $\{d_j(t)\}$, where

$$d_j(t) = \int_0^L \rho^j(a,t)\,da \qquad j = 1, 2, \ldots \tag{11}$$

and the index j denotes the densities resulting from different source terms F_j in (10).

To apply the above algorithm, one must relate the unknown V to the data $\{d_j(t)\}$ in the fashion of equation (2). To this end, (11) can be differentiated to obtain, using (10)

$$\begin{aligned} \dot{d}_j(t) &= \int_0^L \rho_t^j(a,t)\,da \\ &= -\int_0^L V(a)\rho^j(a,t)\,da - \int_0^L \rho_a^j(a,t)\,da + \int_0^L F_j(a,t,\rho_j)\,da \\ &= -\int_0^L V(a)\rho^j(a,t)\,da + h(t) + \int_0^L F_j(a,t,\rho_j)\,da \qquad j = 1, 2, \ldots. \end{aligned} \tag{12}$$

Expanding V as in (4)

$$V(a) = \sum_n a_n \phi_n(a)$$

yields, from (12), the system

$$\sum_n a_n \int_0^L \phi_n(a)\rho^j(a,t)\,da = -\dot{d}_j(t) + h(t) + \int_0^L F_j(a,t,\rho_j)\,da \qquad j = 1, 2, \ldots$$

or

$$M \cdot a = f \qquad (M)_{jn} = \int_0^L \phi_n(a)\rho^j(a,t)\,da$$

corresponding to (5). The resulting expression

$$V(a) = \sum_n \left(M^{-1} \cdot f\right)_n \phi_n(a) \equiv \mathcal{V}\left[d_j, \rho^j\right] \tag{13}$$

is substituted into (10), which is then solved for $\{\rho^j\}$. Finally, V is calculated from $\{\rho^j\}$ through (13).

It is interesting to note that, in this example, M and f are functions of t, while V is time independent. Thus, in the absence of errors, the time dependencies must cancel to have $V = V(a)$ only. If errors are introduced into the problem, the time dependencies may *not* cancel, resulting in a V which also depends on time. This phenomenon will be encountered again in the next example, and addressed in detail later.

3.3. Molecular dynamics

Basic to much of chemistry is the inversion of laboratory data to give underlying fundamental molecular information. A central problem in this regard is determining a given molecule's intramolecular potential energy surface. The relevant evolution law is the time-dependent Schrödinger equation

$$\begin{aligned} i\hbar\frac{\partial\psi}{\partial t} &= \big[K + V(x) + \epsilon(t)\cdot\mu(x)\big]\psi(x,t) \qquad x \in \Omega \subseteq R^n,\ t > 0 \\ \psi(x,0) &= \psi_0(x) \qquad x \in \Omega \end{aligned} \tag{14}$$

where K, the kinetic energy operator, is given by

$$K = \frac{-\hbar^2}{2}\sum_{j=1}^{n}\frac{1}{m_j}\frac{\partial^2}{\partial x_j^2}.$$

The wavefunction $\psi(x,t)$ is complex valued. The function $\epsilon(t)$, representing an external (e.g. laser) field applied to the system, and the function $\mu(x)$, the dipole moment operator, are assumed known. The inverse problem is to determine the potential $V = V(x)$ in (14) from laboratory measurements. Other variants of this problem also arise, but the one posed here suffices to illustrate the methodology.

Denote by $\langle\cdot|\cdot\rangle$ the usual complex L^2-inner product on Ω

$$\langle f|g\rangle = \int_\Omega f^* g\,dx$$

where f^* is the complex conjugate of f. Laboratory data derives from expectation values of a Hermitian operator with respect to ψ; that is, if d is a measurable quantity, then there exists a Hermitian operator O such that

$$d = d(t) = \langle\psi|O\psi\rangle. \tag{15}$$

This operator obeys the Heisenberg equation of motion

$$i\hbar\langle\dot{O}\rangle = \langle[O,K]\rangle + \langle[O,V]\rangle + \epsilon(t)\cdot\langle[O,\mu]\rangle \qquad t > 0 \tag{16}$$

where, for an operator A, $\langle A\rangle \equiv \langle\psi|A\psi\rangle$ denotes the expected value of A. Also, $[A,B] = AB - BA$ denotes the commutator of A with B.

Now, suppose the system in question is exposed to a sequence of external fields $\{\epsilon_j(t)\}_{j=1}^J$, resulting in a sequence of wavefunctions $\{\psi_j\}_{j=1}^J$ obeying (14) for $\epsilon = \epsilon_j$. The corresponding data streams

$$d_j = d_j(t) = \langle O\rangle_j \qquad j = 1,\ldots,J$$

where the subscript j denotes expectation values with respect to ψ_j, are available for inversion to give the potential V. If O does not commute with V, a relation of the form (2) between the unknown V and the data can be obtained from (16)

$$\frac{-i}{\hbar}\langle[O,V]\rangle_j = \dot{d}_j(t) + \frac{i}{\hbar}\langle[O,K]\rangle_j + \frac{i}{\hbar}\epsilon_j(t)\cdot\langle[O,\mu]\rangle_j \qquad j = 1,\ldots,J. \tag{17}$$

Expanding V as in (4)

$$V(x) = \sum_{p=1}^{P} a_p \phi_p(x)$$

the system (17) leads to a matrix equation for the coefficients $a = (a_1, \ldots, a_p)^{\mathrm{T}}$

$$M \cdot a = f \tag{18}$$

where the $J \times P$ matrix M and the J-vector f are given by

$$(M)_{jp} = \frac{-\mathrm{i}}{\hbar} \langle [O, \phi_p] \rangle_j$$

$$f_j = \dot{d}_j(t) + \frac{\mathrm{i}}{\hbar} \langle [O, K] \rangle_j + \frac{\mathrm{i}}{\hbar} \epsilon_j(t) \cdot \langle [O, \mu] \rangle_j$$

and all expectation values in (18) are understood to be taken with respect to the wavefunctions from the system (20) below. With due attention to the meaning of $M^{-1} \cdot f$, one has

$$V(x) = \sum_{p=1}^{P} \left(M^{-1} \cdot f \right)_p \phi_p(x) \equiv \mathcal{V}[d, \psi]. \tag{19}$$

Substitution of V into (14) yields the coupled system

$$\begin{aligned} \mathrm{i}\hbar \frac{\partial \psi_j}{\partial t} &= \left\{ K + \mathcal{V}[d, \psi] + \epsilon_j(t) \cdot \mu \right\} \psi_j \qquad j = 1, \ldots, J \\ \psi_j(x, 0) &= \psi_{0,j}(x) \end{aligned} \tag{20}$$

which is to be integrated to obtain ψ, and, through (19), the unknown V.

Before closing this section on examples, it is important to note that, while the reformulations of these inverse problems are almost identical, the actual implementation of the formal algorithm will depend heavily, in each case, on the specifics of the particular problem and the physical system it models. For example, the precise meaning of the expression (13) in the presence of a singular or near-singular A must be addressed.

4. Stability

Consider a system evolving in time, so that the dynamics are given by a model of the form (1′). As is typical with inverse problems for evolving systems, one must address the stability of a proposed inversion algorithm with respect to errors. Although a general stability analysis for the abstract system in equations (1) and (2) could be undertaken, definite conclusions will be difficult to draw. Here, a special case of the last example is analysed for stability with respect to small errors in the data.

4.1. Stability analysis

Consider the inverse problem for the Schrödinger equation discussed in the previous section, for the case of a diatomic molecule (so that $R^n = R$ in (14)). Suppose that V in (14) is known to be the potential of a harmonic oscillator

$$V(x) = ax^2$$

where the constant a is to be determined. Although this latter assumption is of limited validity for realistic systems, it serves to illustrate the basic stability issues that will arise. The above representation for V may be viewed as an expansion of the form (4), where the basis set $\{\phi_p\}$ consists of a single element $\phi = x^2$. As a special case of data of the form (15), in principle one can measure the average internal energy E of the system as a function of time

$$E = E(t) = \big(\langle K\rangle + \langle V\rangle\big)/\langle\psi|\psi\rangle \qquad t > 0$$

so that (18) takes the form

$$a\langle x^2\rangle = \langle\psi|\psi\rangle E(t) - \langle K\rangle.$$

This results in the non-linear equation

$$\begin{aligned} &\frac{\partial\psi}{\partial t} = \big[K + A[E,\psi]x^2 + \epsilon(t)\cdot\mu(x)\big]\psi(x,t) \\ &\psi(x,0) = \psi_0(x) \end{aligned} \tag{21}$$

where

$$a = A[E,\psi] = \frac{\langle\psi|\psi\rangle E(t) - \langle K\rangle}{\langle x^2\rangle}. \tag{22}$$

Nominally, $\langle\psi|\psi\rangle = 1$, but we must include this term as we will need to consider variations $\psi \to \psi + \delta\psi$ below.

Suppose the data $E(t)$ is contaminated with random noise that is small compared to the true data. The effect of the distribution of this noise on the statistics of the resulting $a = a(t)$ is unclear, given the implicit non-linear dependence of A on E through relation (22). Thus, it is not surprising that the inversion scheme given by (21), (22) may be subject to instabilities with respect to data measurement errors. To reveal the issues involved, we make use of first-order perturbation theory and assume the data signal $E^{\text{data}} = E^{\text{data}}(t)$ is in error by a quantity $\delta E = \delta E(t)$ which is small relative to the true signal

$$E^{\text{data}} = E^{\text{true}} + \delta E. \tag{23a}$$

Here, E^{true} represents the energy generated by the true potential $V^{\text{true}} = a^{\text{true}}x^2$

$$E^{\text{true}} = E^{\text{true}}(t) = \langle K + V\rangle^{\text{true}}/\langle\psi|\psi\rangle^{\text{true}} = \langle\psi^{\text{true}}|(K + V^{\text{true}})\psi^{\text{true}}\rangle$$

where $\langle\psi|\psi\rangle^{\text{true}} = 1$ is employed. Let $a^{\text{inv}} = a^{\text{inv}}(t)$ and ψ^{inv} denote the coefficient and wavefunction, respectively, obtained by applying the inversion scheme (21), (22) to the noisy data E^{data}. The errors in (23a) induce corresponding errors in a^{inv} and ψ^{inv}

$$a^{\text{inv}} = a^{\text{true}} + \delta a \qquad \psi^{\text{inv}} = \psi^{\text{true}} + \delta\psi. \tag{23b}$$

Substitution of (23) into (21) yields, to first order, the following initial value problem for $\delta\psi$

$$\begin{aligned} i\hbar\frac{\partial\delta\psi}{\delta t} &= H\delta\psi + \delta a x^2\psi^{\text{true}} \\ \delta\psi(x,0) &= 0 \end{aligned} \tag{24}$$

where

$$H = H_0 + \epsilon\cdot\mu = K + a^{\text{true}}x^2 + \epsilon\cdot\mu$$

is the true molecular Hamiltonian of the system. From (22), δa, to first order, is given by

$$\begin{aligned} \delta a &= \delta a(\psi^{\text{true}}, \delta\psi; E^{\text{true}}, \delta E) \\ &\approx \frac{\delta A}{\delta\psi}(\psi^{\text{true}}, E^{\text{true}}; \delta\psi) + \frac{\delta A}{\delta E}(\psi^{\text{true}}, E^{\text{true}}; \delta E) \\ &= \frac{2\,\text{Re}\langle\psi^{\text{true}}|\delta\psi\rangle E^{\text{true}}}{\langle x^2\rangle^{\text{true}}} - \frac{2\,\text{Re}\langle\psi^{\text{true}}|H_0\delta\psi\rangle}{\langle x^2\rangle^{\text{true}}} + \frac{\delta E}{\langle x^2\rangle^{\text{true}}} \end{aligned}$$

where

$$\langle x^2\rangle^{\text{true}} = \langle\psi^{\text{true}}|x^2\psi^{\text{true}}\rangle.$$

Defining an operator S by

$$S\phi \equiv \left(\frac{2\langle H_0\rangle^{\text{true}}\,\text{Re}\langle\psi^{\text{true}}|\phi\rangle - \text{Re}\langle\psi^{\text{true}}|H_0\phi\rangle}{\langle x^2\rangle^{\text{true}}}\right)x^2\psi^{\text{true}}$$

(24) becomes

$$\begin{aligned} i\hbar\frac{\partial\delta\psi}{\delta t} &= (H+S)\delta\psi + \frac{\delta E}{\langle x^2\rangle^{\text{true}}}x^2\psi^{\text{true}} \\ \delta\psi(x,0) &= 0. \end{aligned} \tag{25}$$

Thus, noting that H is Hermitian (and thus has a real spectrum), if $\sigma(S)$ represents the spectrum of S at time t, then (25) will be stable if

$$\text{Im}\,\sigma(S) \subseteq (-\infty, 0]$$

for all t sufficiently large. To determine $\sigma(S)$ at a particular time t, note first that

$$\text{Range}(S) \subseteq \{rx^2\psi^{\text{true}} : r \in R\}.$$

Thus, if $\lambda \in C$ and ϕ satisfy

$$S\phi = \lambda\phi$$

then ϕ must have the form

$$\phi = \phi_\alpha = \alpha x^2 \psi^{\text{true}}$$

with $\alpha = \alpha_1 + i\alpha_2$, α_1 and α_2 being real. It is straightforward to show that the corresponding eigenvalue λ_α is given by

$$\lambda_\alpha = \frac{2\alpha^*}{\langle x^2\rangle^{\text{true}}|\alpha|^2}\left\{\langle H_0\rangle^{\text{true}}\,\text{Re}\langle \alpha x^2\rangle^{\text{true}} - \text{Re}\langle H_0 \alpha x^2\rangle^{\text{true}}\right\}$$

and

$$\begin{aligned}\text{Im}\,\lambda_\alpha &= \frac{-2\alpha_2}{\langle x^2\rangle^{\text{true}}|\alpha|^2}\left\{\langle H_0\rangle^{\text{true}}\,\text{Re}\langle \alpha x^2\rangle^{\text{true}} - \text{Re}\langle H_0 \alpha x^2\rangle^{\text{true}}\right\} \\ &= \frac{2}{\langle x^2\rangle^{\text{true}}|\alpha|^2}\left\{\alpha_1\alpha_2\left(\text{Re}\langle H_0 x^2\rangle^{\text{true}} - \langle H_0\rangle^{\text{true}}\langle x^2\rangle^{\text{true}}\right) - (\alpha_2)^2\,\text{Im}\langle H_0 x^2\rangle^{\text{true}}\right\}.\end{aligned} \tag{26}$$

Since $|\psi^{\text{true}}\rangle$, H_0 and x^2 are independent of α, it is clear from (26) that there may exist values of α for which $\text{Im}\,\lambda_\alpha > 0$. Consequently, the inversion algorithm (21), (22), is *not* unconditionally stable with respect to errors in the data measurements. A robust solution to this problem needs to be developed, and some factors contributing to the possible instability are addressed below.

4.2. Asymptotic tracking of data

Observe that the relation (22) forces the potential coefficient $a^{\text{inv}} = a^{\text{inv}}(t)$ to agree with the (noisy) data $E^{\text{data}}(t)$ *at each time* t. In an effort to improve the stability properties of the algorithm, one may consider relaxing this condition by requiring only that the coefficient $a^{\text{inv}}(t)$ generates energies $E^{\text{inv}}(t)$ which approach the data $E^{\text{data}}(t)$ at a prescribed rate in time. Mathematically

$$\frac{\text{d}}{\text{d}t}\left\{E^{\text{inv}}(t) - E^{\text{data}}(t)\right\} = -c(t)\left\{E^{\text{inv}}(t) - E^{\text{data}}(t)\right\} \tag{27}$$

where the function $c(t)$, with $c(t) > 0$, $\forall t$, controls the rate of tracking. This idea is inspired by the technique of asymptotic tracking, as applied to non-linear control theory (see, e.g. [10]). Related techniques have been employed recently in the context of learning control of robotics [8] and inverse quantum-mechanical control [6].

Such behaviour can be effected by replacing the functional relation (22) by starting with the relation

$$E^{\text{inv}} = \langle K\rangle^{\text{inv}} + \tilde{a}^{\text{inv}}\langle x^2\rangle^{\text{inv}} \tag{28}$$

where $\tilde{a}^{\text{inv}}$ represents the inverse solution resulting from the algorithm to be developed in this section (equation (30) below). The relation (28) is then substituted for $E^{\text{inv}}(t)$ in the right-hand side of (27) to obtain

$$\tilde{a}^{\text{inv}} = \tilde{A}[E,\psi](t) = \frac{1}{\langle x^2\rangle}\left\{E^{\text{data}}(t) - \langle K\rangle - \frac{1}{c(t)}\left[\dot{E}^{\text{inv}}(t) - \dot{E}^{\text{data}}(t)\right]\right\} \tag{29}$$

where the overdot denotes time differentiation. Note that in the case of noise-free data, $E^{\text{inv}}(t) = E^{\text{data}}(t)$, so that (29) reduces to the original relation (22).

The Heisenberg equation (16) can be combined with (28) to obtain

$$\dot{E}^{\text{inv}}(t) = \dot{\tilde{a}}^{\text{inv}}\langle x^2\rangle^{\text{inv}} - \frac{\mathrm{i}}{\hbar}\epsilon(t)\langle[K,\mu]\rangle^{\text{inv}}$$

so that (29) becomes

$$\dot{\tilde{a}}^{\text{inv}} + c(t)\tilde{a}^{\text{inv}} = \frac{1}{\langle x^2\rangle^{\text{inv}}}\left\{\left[\dot{E}^{\text{data}}(t) - \frac{\mathrm{i}}{\hbar}\epsilon(t)\langle[K,\mu]\rangle^{\text{inv}}\right] + c(t)\left[E^{\text{data}}(t) - \langle K\rangle^{\text{inv}}\right]\right\}. \tag{30}$$

The inversion algorithm now proceeds by solving (21) and (30) as a coupled system of differential equations.

4.3. Tracking time averages of data

Going a step further, in the case where the data is contaminated with mean-zero random noise, it may be more desirable to track the *statistical mean* of the data as a function of time. Such an average acts as a filter to help remove the noise in the data. Denoting the time average of a function $f(t)$ by

$$\bar{f}(t) = \frac{1}{t}\int_0^t f(s)\,\mathrm{d}s$$

it follows that

$$\frac{\mathrm{d}}{\mathrm{d}t}\{\bar{f}(t)\} = \frac{1}{t}\{f(t) - \bar{f}(t)\}.$$

Beginning with the relation

$$\frac{\mathrm{d}}{\mathrm{d}t}\{\bar{E}^{\text{inv}}(t) - \bar{E}^{\text{data}}(t)\} = -c(t)\{\bar{E}^{\text{inv}}(t) - \bar{E}^{\text{data}}(t)\} \tag{31}$$

analogous to (27), equation (30) is replaced by the integral equation

$$\begin{aligned} a(t) + \frac{1}{\langle x^2\rangle^{\text{inv}}(t)}\left[c(t) - \frac{1}{t}\right]\int_0^t a(s)\langle x^2\rangle^{\text{inv}}(s)\,\mathrm{d}s \\ = \frac{1}{\langle x^2\rangle^{\text{inv}}(t)}\left[E^{\text{data}}(t) - \langle K\rangle^{\text{inv}}(t)\right] \\ + \frac{t}{\langle x^2\rangle^{\text{inv}}(t)}\left[c(t) - \frac{1}{t}\right]\left[\bar{E}^{\text{data}}(t) - \langle\bar{K}\rangle^{\text{inv}}(t)\right]. \end{aligned} \tag{32}$$

A suitable form for the damping function $c(t)$ must be specified, and there is considerable flexibility in this choice. To this end, let $\{t_j\}_{j\geqslant 1}$ be a discretization of the time variable t, and suppose the data is given by $\{E_j^{\text{data}} = E^{\text{data}}(t_j)\}_{j\geqslant 1}$. The desirability of tracking the average of the data rather than the data values themselves is based on the strong law of

large numbers, which asserts that the statistical mean of the noise converges to its theoretical mean, which is assumed to be zero. Thus, if the noise is uncorrelated, then

$$\lim_{t\to\infty}\left(\bar{E}^{\text{noisy}}(t)-\bar{E}^{\text{true}}(t)\right)=0 \tag{33}$$

permitting the algorithm to track a 'signal' which converges to the true signal. If $\bar{E}^{\text{noisy}}(t)$ is tracked too fast (e.g. before the noise has sufficiently averaged away), then the algorithm is once again tracking noisy data, and the same instability issues arise. Consequently, the damping function $c(t)$ should be chosen to produce a tracking rate which is *slower* than the rate that the statistical mean of the noise converges to zero. However, the law of large numbers gives no information on this convergence rate. The definitive result in this regard is the law of the iterated logarithm from classical probability theory. A proof of the following version of this result can be found in the monograph by Chung [4, p 232].

Theorem. Law of the iterated logarithm. Let $\{X_j : j \geqslant 1\}$ be a sequence of independent identically distributed mean-zero random variables with common variance σ^2, and assume each X_j has a finite second moment. Let

$$\bar{X}_J=\frac{1}{J}\sum_{j=1}^{J}X_j.$$

Then, with probability one

$$\limsup_{J\to\infty}\frac{\sqrt{J}\bar{X}_J}{\left[2\sigma^2\log\log(\sqrt{J}\sigma)\right]^{1/2}}=1$$

and

$$\liminf_{J\to\infty}\frac{\sqrt{J}\bar{X}_J}{\left[2\sigma^2\log\log(\sqrt{J}\sigma)\right]^{1/2}}=-1.$$

So, with probability one, $\bar{X}_J$ converges to zero on the order of

$$\sqrt{\frac{\log\log J}{J}}\qquad \text{as } J\to\infty. \tag{34}$$

Hence, $c(t)$ should effect the convergence in (33) at a rate slightly *slower* than (34). For any $\alpha\in(0,1)$, this can be achieved by selecting $c(t)$ to be

$$c(t)=c(t_J)=\frac{\alpha}{2J}. \tag{35}$$

To see this, first note that, from (31)

$$\bar{E}^{\text{inv}}(t_J)-\bar{E}^{\text{data}}(t_J)=O\left(J^{-\alpha/2}\right)$$

where

$$\bar{E}^{\text{inv}}(t_J)=\frac{1}{J}\sum_{j=1}^{J}E^{\text{inv}}(t_j)$$

and likewise for $\bar{E}^{\text{data}}(t_J)$. It only remains to show that $J^{-\alpha/2}$ converges to zero at a slower rate than that indicated in (34). Indeed, L'Hôpital's rule shows that for any α, $0<\alpha<1$

$$\lim_{J\to\infty}J^{\alpha-1}\log\log J=0$$

and hence proves the assertion on the rate of convergence.

5. Numerical example

The practical implementation of the present algorithm will, of course, depend on the complexity of the physical system under consideration. It is not our intention here to test the limits of its applicability, but rather to demonstrate its use in one particular case. As a simple illustrative example, consider the harmonic oscillator inverse problem introduced in the previous section. The particular model system studied represents a diatomic molecule. We seek to recover the potential curve from the data $\{E_j^{\text{data}} = E^{\text{data}}(t_j)\}$ by employing the stabilized inversion algorithm (21), (32). The potential curve $V(x)$ to be recovered is taken to have the form

$$V(x) = \tfrac{1}{2}m\omega^2 x^2 \tag{36}$$

where m is the reduced mass of the system and ω is the frequency of the oscillator. For the purposes of this simulated inversion, the dipole moment function $\mu(x)$ of the system is chosen to be

$$\mu(x) = \mu_1 x \tag{37}$$

and the external field $\epsilon(t)$ is taken as

$$\epsilon(t) = \Theta(t) L \sin(\sigma t) \tag{38}$$

where Θ is a smooth cut-off function which simulates the external field $\epsilon(t)$ being turned off after a certain time. In the present example, $\Theta(t)$ is chosen to be the C^1-function given by

$$\Theta(t) = \begin{cases} 1 & 0 \leqslant t \leqslant \tau_1 \\ 0.5\big(1 + \cos[\pi(t-\tau_1)/(\tau_2-\tau_1)]\big) & \tau_1 < t < \tau_2 \\ 0 & t \geqslant \tau_2 \end{cases}$$

where $\tau_1 = 10\,000$ and $\tau_2 = 20\,000$ in atomic units. The following values for the constant parameters appearing in (36) and (37) were obtained from [9, p 340], and are given in atomic units

$$m = 5.05 \times 10^4 \qquad \omega = 0.001\,7509 \qquad \mu_1 = 0.488.$$

The period T of the harmonic oscillator is

$$T = 3588.55.$$

The parameters for the external field $\epsilon(t)$ in (38) are chosen to be

$$L = 0.001 \qquad \sigma = \omega = 0.001\,7509.$$

From (36), the coefficient a to be recovered has the value

$$a = a^{\text{true}} = \tfrac{1}{2}m\omega^2 = 0.077\,4077.$$

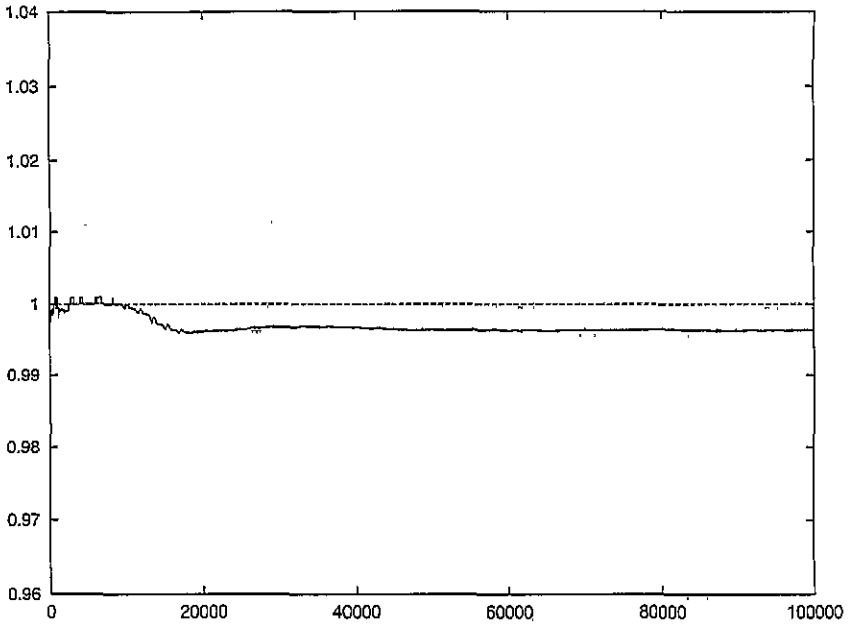

Figure 1. The normalized inverse solution $a^{\text{ens}}(t)/a^{\text{true}}$ as a function of time.

Synthetic data $E^{\text{true}}(t)$ are generated from a^{true} using the split operator method of Feit *et al* [5]. The data is then contaminated with 10% mean amplitude Gaussian noise.

The inversion proceeds by propagating (21) and (32) as a coupled system, taking $c(t)$ in (32) to have the form (35) with $\alpha = 0.9$. The solution of (32) requires an initial value a_0 for $a(t)$, taken here to be $a_0 = a^{\text{true}}$. It is worth noting that, after many numerical experiments in which a number of different values of a_0 were used, it was determined that the algorithm can tolerate a certain level of uncertainty in the value of a_0. This is a result of the relatively short transient involved, during which time the wavefunction does not change appreciably.

The system is propagated for approximately 28 periods of the true potential, or 100 000 atomic time units. Because of the probabilistic nature of the algorithm, this simulated inversion is repeated, using a number N of different noisy data sets ($N = 50$ in this case). The inverted coefficients $\{a_n = a_n(t)\}_{n=1}^{N}$, resulting from these individual runs, are then combined to produce an ensemble average $a^{\text{ens}}(t)$ of the inverted coefficients

$$a^{\text{ens}}(t) = \frac{1}{N}\sum_{n=1}^{N} a_n(t).$$

Figure 1 shows the normalized value $a^{\text{ens}}(t)/a^{\text{true}}$ of this ensemble coefficient plotted against time. It is seen that the ensemble average coefficient a^{ens} converges to a value that is within 0.4% of the true value a^{true} ($a^{\text{ens}} \approx 0.077\,6781$). In an effort to confirm the convergence in this simulation, the inversion algorithm was permitted to continue for another 300 000 time units. The value of a^{ens} did not change significantly during this period. The ensemble standard deviation $s_N(t)$, given by

$$s_N(t) = \left(\frac{1}{N-1}\sum_{n=1}^{N}\left(a_n(t) - a^{\text{ens}}(t)\right)^2\right)^{1/2}.$$

was computed to be of the order of 3%. The energies generated by the final value of a^{ens} were found to lie within 0.2% of the noise-free input data.

The fact that, in this numerical example, the ensemble average coefficient a^{ens} converges to a value which differs (slightly) from the true value a^{true} has two likely sources. First is the practical matter that, since the noise corresponds to one particular finite set of mean-zero deviates, its contribution to the error need not average to zero itself. Second, and this is the main source, it must be remembered that the inversion procedure depends non-linearly on the system wavefunction ψ, which in turn depends on the value of the inverted coefficient $a^{\text{inv}}(t)$. Thus, if $a^{\text{inv}}(t)$ differs from a^{true}, then ψ^{inv} will differ from ψ^{true}. Furthermore, since ψ^{inv} enters non-linearly, one cannot expect the effects to cancel completely in the ensemble average. As a larger ensemble of data is included, one should find that the asymptotic result

$$\lim_{t\to\infty} a^{\text{inv}}(t) = a^{\text{true}}$$

holds.

To further illustrate the necessity of the stabilization procedure used in the development of the inversion scheme (21), (32), the unstabilized algorithm (21), (22) was implemented with the input data contaminated with 10% noise. The results of this exercise show that the unstabilized algorithm diverged after about 15 000 time units. Thus it is clear that, even in this simple example, stabilization is an important issue for this inversion method.

We close this example section by noting that, in practice, one would typically pre-average laboratory data signals, in an effort to minimize the effects of measurement imprecision. This is in contrast to the present example, in which the 'raw' data is used directly as input to the inversion algorithm, and the scheme is given the task of minimizing the effects of the noise. Thus, the present example can be considered as a stringent test for the algorithm, requiring more stability than may be needed in practice. In this regard, the remarkable stability inherent in the results of this example is encouraging.

6. Conclusions

In this paper we have presented a general algorithm for the inversion of physical systems. The potential broad applicability of this algorithm has been demonstrated through representative inverse problems from different scientific disciplines. The issue of stability in the presence of measurement imprecision was addressed in the context of an example problem from quantum dynamics. A stabilization procedure, based on asymptotic tracking, was proposed. Our results for this example problem show that the method is remarkably successful in producing a stable inverse solution for the potential that is consistent with the input data. A major advantage of our method is the fact that it produces a *direct* inversion of the data, in contrast to computationally expensive iterative schemes. This makes the method potentially quite attractive for the study of higher-dimensional systems, where the numerical computations are more expensive. A second advantage of this method is its potential broad applicability to a wide range of inverse problems. A much more thorough study of the method is needed, including further illustrations, to establish its full utility. At a minimum, with the methodology introduced in this paper, we hope to have established a first step in an alternative means for the inversion of physical systems.

It should be noted that the model example presented in the last section only serves the purpose of illustration. In general, one cannot expect to know *a priori* the functional form of the unknown w of equation (1). Consequently, the choice of basis in the expansion (4)

becomes an issue, and one would expect different choices to lead to different performance characteristics in the implementation of the algorithm. For example, it may be advantageous in a particular application to expand w as a collection of delta functions, thereby effecting discretization. The issue of choosing the 'best' basis expansion for w should be addressed in the context of the particular application being considered.

As with any general inversion scheme, the algorithm presented here should be applied with discretion and using physical and mathematical judgement.

One cannot expect to determine the true w from arbitrary data, as this often leads to non-trivial nullspaces in the inversion. For example, in the quantum mechanical case it is known that, at any particular time, data of the form (15) contain no information on the unknown potential $V(x)$, except (possibly) in the regions where $|\psi(x,t)|^2$ is significant. Thus it is unrealistic to attempt to determine $V(x)$ outside of these regions from the given data. Rather than a shortcoming of the present method, this is simply a reflection of the fact that for realistic data, inverse problems are typically ill-posed. A useful inversion method should allow for the retrieval of the relevant information that *is* contained in the data, while safeguarding against the extraction of erroneous results during the inversion process. Designing an algorithm to achieve the latter objective depends heavily on the special properties of the particular physical system under consideration. The inverse in equation (3) can be regularized by, for example, smoothness criteria on w to deal with singularities due to an inadequate data set. Such design concerns for the present algorithm, as applied to the quantum-mechanical example of section 3, will be explored in future work.

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