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To cite this article: William Rundell 2024 Inverse Problems 40 125013

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IOP Publishing

Inverse Problems

Inverse Problems **40** (2024) 125013 (15pp) https://doi.org/10.1088/1361-6420/ad904c

Recovery of a coefficient in a diffusion equation from large time data*

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Received 14 April 2024; revised 23 September 2024
Accepted for publication 8 November 2024
Published 20 November 2024

Abstract
This paper considers the determination of a spatially varying coefficient in a parabolic equation from time trace data. There are many uniqueness theorems known for such problems but the reconstruction step is severally ill-posed: essentially the problem comes down to trying to reconstruct an analytic function from values on a strip. However, we look at an even more restricted data where the measurements are not made on the whole time axis but only for large values adding further to the ill-conditioning situation. In addition, we do not assume the initial state is known. Uniqueness is restored by making changes to the boundary condition, in particular, to the impedance parameter, for each of a series of measurements. We show that an undefined implementation of the above paradigm leads to both uniqueness and an effective reconstruction algorithm. Extension is also made to the case of fractional model and to replacing the parabolic equation with a damped wave equation.

Keywords: inverse problems, coefficient recovery, parabolic, subdiffusion and wave equations

1. Introduction

The recovery of unknown spatially-dependent coefficients in a parabolic equation from additional measurements is a ubiquitous inverse problem driven by numerous applications. One canonical example is the recovery of the potential coefficient $q(x)$ in a parabolic equation setting

$$
\begin{aligned}
&u_t - \triangle u + q(x)\,u = 0 \qquad x \in \Omega, \\
&Bu = \frac{\partial u(x,t)}{\partial \nu} + \beta u = 0 \qquad x \in \partial\Omega, \quad t > 0, \\
&u(x,0) = u_0(x) \qquad x \in \Omega.
\end{aligned} \tag{1}
$$

* This work was supported in part by the National Science Foundation through award DMS-2111020.

Here the boundary impedance parameter β and the initial condition $u_0(x)$ are given.

This particular problem dates to the early 1980's but we will stipulate a sometimes very reasonable physical but mathematically restrictive condition on our measurement data that requires a novel approach to its solution.

We could also consider the non-homogeneous case of including known right-hand side functions $f(x,t)$ in the differential equation and $g(t)$ in the boundary condition in (1) but this would add further detail rather than salient features and we prefer to take the 'less is more' approach. As we note below, we could also replace the elliptic part of the operator by $-\big(a(x)u_x\big)_x$ where $a(x)$ is a conductivity or instead consider a $d(x)u_t$ term. Then in the resulting inverse eigenvalue problem our potential can be converted from $d(x)$ by the Liouville transform, [14].

Given the value of $q(x)$, equation (1) constitutes a well-posed problem for $u(x,t)$ and the inverse problem turns this around and seeks to impose additional information on $u(x,t)$ that allows the recovery of q. Two common cases are *final time data* $u(x,T) = h(x)$ for $x \in \Omega$ and *time trace data* $u(x_0,t) = f(t)$ for $t > 0$ for some point $x_0 \in \overline{\Omega}$ and, typically, $x_0 \in \partial\Omega$. These are quite different inversion problems giving rise to distinctly different results.

In the former case we have a map $h \to q$ that is defined on Ω and allows, for example, the construction of a fixed point scheme based on

$$q(x) = \mathbf{T}[q] := \big(u_t(x,T;q) - \triangle h\big)/h \tag{2}$$

where we have projected the equation onto the line $t = T$. Under suitable conditions, a unique fixed point can be shown, See, for example, [3, 12, 13, 19]. For a given value of $q(x)$, lying in $C^{0,\gamma}(\Omega)$, $0 < \gamma < 1$, the solution of the direct problem $u \in C^{2+\gamma}$ and (2) is consistent from a space-to-space perspective. Thus our data h should lie in $C^{2+\gamma}$ and the inverse problem is mildly ill-conditioned with a two derivative loss $h \to q$. The drawback in the above is the necessity of taking interior measurements over all of Ω which most often is not feasible from an experimental standpoint and time-trace data case is more commonly used in applications.

In this latter case we have the solution representation

$$u(x,t) = \sum_1^\infty a_n e^{-\lambda_n t}\phi_n(x) \tag{3}$$

where $\{\lambda_n\}$, $\{\phi_n\}$ are the eigenvalues and eigenfunctions of the operator $-\triangle + q$ on Ω subject to the boundary conditions $Bu = 0$ and $\{a_n\}$ are the Fourier coefficients of the initial data $u_0(x)$ with respect to the basis $\{\phi_n\}$. Of course these are unknown as they depend on q. The usual attack in one space dimension is to convert to an inverse Sturm–Liouville problem for the unknown potential q. If we evaluate (3) at (say) the right hand boundary point $x = 1$ then we obtain the relation

$$f(t) := u(1,t) = \sum_1^\infty a_n e^{-\lambda_n t}\phi_n(1). \tag{4}$$

The measured $f(t)$, in (4) is a Dirichlet series with the components $\{\lambda_n\}_{n=1}^\infty$, $\{a_n\phi_n(1)\}_{n=1}^\infty$. Knowledge of this function on any interval allows the recovery of the spectrum $\{\lambda_n\}$ and endpoint values $\phi_n(1)$ assuming the initial condition $u_0(x)$ is given, see lemma 3.1 in section 3. From this, standard results for the inverse Sturm–Liouville problem show this pair is sufficient to uniquely determine $q(x)$ in this one space-dimensional setting. This approach was first proposed by Pierce, [11] and has formed the basis of numerous works over the last 40 years: see, for example, [4] and references cited below.

Here we also take this aspect of the problem but do so under severe restrictions on the measured data: the often realistic physical situation when one can only make a small and discrete number of time measurements within a relatively narrow interval and *only* for sufficiently large values. We will invoke a similar inversion theorem for Dirichlet series together with a result from [10] to prove uniqueness. With this we then demonstrate how a relatively small number of time measurements taken at only large time values and for a selection of impedance values $\{\beta_k\}$ can lead to an effective reconstruction process.

However, the ill-conditioning now is considerably different from the case of spatial data $u(x,T)$. While the inversion $\{\lambda_n, \phi_n(1)\} \to q(x)$ is only mildly ill-conditioned, [14, 15], the inversion of the Dirichlet series for the weights $\{a_n\}$ and the exponents $\{\lambda_n\}$ is severely ill-posed since the eigenvalue asymptotic behaviour is $\lambda_n = n^2\pi^2 + \bar{q} + O(\ell^2)$. Clearly, large or even modest values of t lead to the terms of the series having *effectively* infinitesimal values. Thus any optimal interval should include very small time values. This is not a question of non-uniqueness but of the severe ill-conditioning inherent in inverting the Dirichlet series representation for $f(t)$ to obtain $\{a_n\}$. Even if an alternative to an inverse spectral approach is taken the ill-conditioning of the map $u(1,t) \to q$ is intrinsic and remains.

It is worthy of a remark here that recovery of just the eigenvalues $\{\lambda_n\}$ is not in general sufficient to determine $q(x)$. One requires two different spectra $\{\lambda_n, s_n\}$ arising from different boundary conditions at $x = 1$; that is the spectrum arising from two different values of β although a single spectrum suffices if q is known to be symmetric about the midpoint, $q(x) = q(1-x)$. This is the landmark theorem of Borg's 1946 paper, [1]. A few years later Levinson gave a much shorter and elegant proof, [9]. A single time-trace measurement and initial condition provides a spectrum and using the initial condition provides so-called *norming constants*, as noted above. Uniqueness of the $q(x)$ from this combination is the result of another early seminal paper on the topic by Gel'fand and Levitan in 1951, [2]. In the time-trace recovery problem stated above these norming constants are obtained from the sequence $\{a_n\}$ which in turn is derived from the initial data u_0. The above arguments hold only in a single space dimension and there is no multi-dimensional analogue as the multiplicity of eigenvalues (amongst other things) in this case destroys the uniqueness results.

Our solution and the main novelty in the paper is to allow a change in impedance value β at the right-hand endpoint and then make measurement of $u(1,t) = u(1,t,\beta)$ under these conditions. While the uniqueness result to be stated requires all values of β lying in a non-empty interval or having a finite accumulation point, we will see that from a reconstruction perspective that taking a relatively small discrete sample of values suffices. We will show how this can be achieved by using multiple experiments. As an offset to this one will be able to maintain *effective* uniqueness and reconstruction with just a pair of measurement points $u(1,t_j)$, for each experiment. Of course, with any experimental error in the data $f(t)$ additional points will help to a great extent and with experimental error in the data $f(t)$ some oversampling is necessary.

We now clarify the meaning of 'large times.' The mathematical version of the heat equation $u_t - c\triangle u = 0$ sets the diffusion constant c to be unity. This constant c couples the time and space dimensions and in almost all applications is far from unity. For example, modelling the diffusion of a molecule in the gas phase gives a c typically in the range 10^{-6} to 10^{-5} meters^2/sec; while in the liquid phase it would be from 10^{-10} to 10^{-9} meters^2/sec. Thus taking a time measurement at say $T = 1$ second in the version with $c = 1$ corresponds to about a week in the physical version. In this sense (mathematical) time values even in the range $0.1 - 1$ can be considered as 'large times' from a physical context. An entirely analogous situation holds for the wave equation and recovering the wave speed $c(x)$ instead of $q(x)$ (or fact recovering the 'effective potential' $Q(x)$ then using the Liouville transform to translate Q into

$c(x)$. Wave speeds can vary over quite considerable ranges from a fraction of a meter/second for water waves to 300 meters/second for electromagnetic waves.

On a broader front, the Liouville transform allows each of the equations $-\phi'' = \lambda_n \rho(x)\phi$ and $-\big(a(x)\phi'\big)' = \lambda_n\phi$ to be transformed into the canonical 'potential form' involving just $q(x)$. Thus the coefficient to be determined in the parabolic setting could be a conductivity or a specific heat in place of the stated potential in equation (1). This is possible here due to the fact that we have time trace data. If we replace the elliptic operator L in potential form with $q(x)$ by one with an unknown conductivity $c(x)$, so that $Lu = \big(c(x)u'\big)'$ then the fixed point analysis mentioned earlier for equation (2) and spatial final time data becomes much more complex.

In this paper we will also make the restriction of a single spatial variable. We will assume that the only data that can be measured are time values of the solution at a boundary point and that these measurements can only be taken for very large times. Specifically, we will assume that the sampled points are taken from the interval $T - L \le t \le T$ where L is significantly smaller than T and that the number of sampled points m is also small—in the low double digits range. In the reconstructions shown in section 6 we used $T = 1$ and $L = 0.1$ although L could have been taken somewhat smaller to almost the same effect. We will *not* assume the initial condition $u_0(x)$ to be known. This is an important feature of the approach—both from a mathematical and physical perspective.

Of course, recovering a general potential $q(x)$ from this is impossible from only a single experiment. Thus for uniqueness we assume that we are able to change the boundary impedance parameter $\beta = \beta_j$ over an infinite range of j and we will show that this will suffice to prove the unique recovery of the potential $q(x)$. In addition, we will indicate how this approach can lead to a reconstruction algorithm based on the above stated range of data measurements $u(1,t;\beta)$ and can effectively approximate $q(x)$ by a relatively small sampling of measurements $u(1,t;\beta)$ for different $\{\beta_j\}$.

In the final section of the paper we also briefly consider similar models that can benefit from the same reconstruction paradigm. The first is the subdiffusion case where the pde in (1) is replaced by $\partial_t^\alpha u - \triangle u + q(x)u = 0$ where ∂_t^α denotes the fractional derivative of Djrbashian type: that is, the usual time derivative is taken followed by an Abel fractional integral operator, [5, 7]. The second, the damped wave equation $u_{tt} - c(x)u_{xx} + du_t = 0$, where the wave speed $c(x)$ has to be recovered from time-trace data. The solutions also decay exponentially for large time if $d > 0$ and the problem can again be converted to one of inverse Sturm–Liouville type; in this case for recovering $c(x)$.

2. An Inverse Sturm–Liouville uniqueness theorem

The following result can form the core for a variety of spatially varying undetermined coefficient problems for time-dependent equations: parabolic, hyperbolic and subdiffusion equations, under the premise that we can (only) measure boundary time trace information for very large times but with the limitation to a single space variable. Here is the setting in the case of a potential $q(x)$ although the Liouville transform will allow the inclusion of other basic types.

Consider the eigenvalue problem

$$-y'' + q(x)y = \lambda y \qquad y(0) = 0, \quad y'(1) + \beta y(1) = 0. \tag{5}$$

The usual Sturm–Liouville question is to be given the function $q(x)$ and the number β and from this to determine the spectrum $\Lambda = \{\lambda_n\}$. As noted earlier, there are numerous versions of the isl problem depending on what is measured. A slightly different version is the following, [10]

Theorem 2.1. *Let q_1 and $q_2 \in L^2(0,1)$ satisfy equation (5). Fix j a positive integer and take a sequence $\{\beta_k\}$ of distinct real numbers. If $\lambda_j(q_1,\beta_k) = \lambda_j(q_2,\beta_k)$ for $k = 1,2,\ldots$ then $q_1(x) = q_2(x)$.*

In other words, the potential q can be determined uniquely from measuring an eigenvalue of fixed index for an infinite sequence of impedance values β_k on one boundary point while keeping the condition at the other boundary fixed. A few remarks are in order here.

Firstly, the proof uses analyticity of the eigenvalues on the parameter β and in fact uniqueness holds for any infinite sequence of distinct values $\{\beta_j\}$ with an accumulation point since compactness then shows there must be a limit point. However, a sequence $\{\beta_j\}$ confined to a narrow interval is far form optimal and choosing the values $\{\beta_j\}$ to encompass a maximal range between Dirichlet–Neumann and Dirichlet–Dirichlet conditions leads to superior conditioning of the inversion process.

Secondly, we could also set the left hand condition in (5) to be of Neumann type, or indeed of impedance form $y'(0) - \alpha y(0)$ for any fixed α, $0 \leqslant \alpha < \infty$.

Combining this result with Borg's original two spectral version gives a convenient way to look at the inverse spectral uniqueness question. Let $\lambda_{k,\beta}$ denote the eigenvalues corresponding to $-u'' + q(x) = \lambda_{k,\beta}$, with either $u(0) = 0$ or $u'(0) = 0$ together with $u'(1) + \beta u(1) = 0$ and consider λ indexed as an array with rows formed from the constant k indices and columns representing the β values in a monotonic order with an accumulation point. Then the eigenvalues taken from any two distinct columns or from any row uniquely determines q. This observation in fact contains the essence of the proof of theorem (2.1) used in [10].

In our case due to theorem (2.1) we do not need to obtain the $\{b_n\}$, which provides the norming constants for the Gel'fand-Levitan approach, only the $\{\lambda_n\}$ sequence as a function of β. Hence we do not require knowing the initial condition $u(x,0)$. This is a substantial and possibly critical benefit since as we are measuring only for later times there is the likelihood that a measurement of the initial distribution is unobtainable.

Further, for a uniqueness result we need only measure $g(t)$ over an arbitrary small interval due to analyticity of the Dirichlet series representing this function. As a more practical matter we will sample discrete points $\{t_k\}$ within this interval and perform a least squares fit to these measurements. We will address this point in the next section.

3. Recovery of the spectral values $\{\lambda_n\}$ from time-trace data

We begin by stating the unique recovery result for the components of a Dirichlet series from a measurement of values over any interval.

Lemma 3.1. *Let f(t) be given as in (4) where $\{a_n\} \in \ell^2$ and the sequence $\{\lambda_n\}$ has nonnegative entries. Then f(t) measured over any non-empty interval uniquely determines the sequences $\{a_n\}$, $\{\lambda_n\}$.*

The proof is very standard. The conditions on $\{\lambda_n\}$ guarantee convergence for $t > 0$ and the series represents an analytic function on this set. Thus knowledge of f over any nonempty interval (or even for a sequence $\{t_j\}$ with a finite accumulation point) determines f over the whole positive line. Then we may take the Laplace transform $f(t) \to \hat{f}(s)$ to obtain $\hat{f}(s) = \sum_1^\infty \frac{b_n}{s-\lambda_n}$.

Then knowing $\hat{f}(s)$ allows recovery of $\{b_n\}$ and $\{\lambda_n\}$ identifying the latter as the poles of $\hat{f}(s)$ on the positive real axis.

For each impedance value β this series will contain eigenvalues $\lambda_1(\beta), \lambda_2(\beta), \ldots, \lambda_k(\beta), \ldots$ where $\lambda_k(\beta)$ corresponds to the k^{th} frequency for this fixed value of β. The lowest value will (shifted by an amount equal to the mean of q) lie in the interval $(\frac{\pi}{2}^2, \pi^2)$, the second in $(\frac{3\pi}{2}^2, 4\pi^2)$, and so on. The question then becomes how many levels of these k can be extracted from inverting the series to obtain $\lambda_k(\beta)$?

Overall, it makes sense to concentrate on finding the lowest eigenvalue $\lambda_1(\beta_j)$ for each impedance value $\{\beta_j\}$. If we look directly at the solution itself and consider only the leading term of λ_j then: for a time value $t_1 = T$, $e^{-\lambda_1 t_1}$ will be approximately the same magnitude as $e^{-\lambda_2 t_2}$ when $4t_2 = t_1$. Thus the expected ratio between the first and second range in k is approximately $e^{-4} \approx 0.018$ and the first and third range it is $e^{-9} \approx 10^{-4}$. The second range difference of these is likely to be close to the measurement error in the time trace data $g(t)$ and the third almost certainly there and hence neglible.

Given these values we can for all practical purposes exclude the third and higher eigenvalues corresponding to the index k. Thus we have two remaining possibilities: we can recover only the lowest eigenvalue $\lambda_k(\beta)$ with $k = 1$ for each β value used, or we can attempt to recover $\lambda_k(\beta)$ with $k = 1, 2$.

In the first case, for each β the representation $g(t) = a_1 e^{-\lambda_1(\beta)t}$ gives $\log g_\beta(t) = \log a_{1j} - \lambda_1 t$ and from which we can recover λ_1 from two measurement values, in fact discarding the a_{1j} since this is not needed for our spectral recovery of λ. In the second case $g(t) = a_1 e^{-\lambda_1(\beta)t} + a_2 e^{-\lambda_2(\beta)t}$ and four measurement values are needed for the values $\{a_{i,j}\}, \{\lambda_{i,j}(\beta_j)\}, i = 1, 2$ although once again the values corresponding to the initial condition can be neglected. We thus have

Theorem 3.1. *Let q_1, $q_2 \in L^2(0,1)$ and let $u = u(x,t;q_i,\beta)$ satisfy (1). Then if we ignore all frequencies above the ground states $\lambda_1(\beta)$ then for two time values t_i, $i = 1, 2$ we have $u(1,t_i;q_1,\beta) = u(1,t_i;q_2,\beta)$ for an infinite sequence of distinct β values in $[0,\infty)$ then $q_1 = q_2$. If we also seek to obtain the second lowest states then at least four time values $\{t_i\}_{i=1}^4$ are required.*

Later we will see that there is a tangible advantage in being able to recover $\{\lambda_k(\beta)\}$ for $k > 1$ if this is feasible from our data. It means that the condition number of the next stage inversion of converting $\{\lambda\}$ into $q(x)$ is considerably reduced. An quantitative measure of this will be seen in figure 4 in section 7.

In our reconstruction to be shown in section 6 in order to allow for measurement error in the time trace $g(t)$ arising from our direct solver we just used the lowest eigenvalue case above, taking in fact 5 sample time points for each β-run. Then a simple least squares fit was used to estimate our ground state eigenvalues $\{\lambda_1(\beta)\}$.

In the subdiffusion case involving a fractional operator to be discussed in the last section we can in fact feasibly use this process to include higher indices $k > 1$ in our $\lambda_k(\beta)$ values.

4. Determining the Cauchy values f, K from the eigenvalues

For the moment we assume that only the lowest eigenvalue (and hence eigenfunction) is involved and will use the subscript index to denote the eigenvalue/eigenfunction arising from the j^{th} value of the impedance β_j. These eigenfunctions $\{\phi_j(x;\lambda_j,\beta)\}$ satisfy $\phi_j(0) = 0$,

$\phi_j'(1) + \beta(j)\phi_j(1) = 0$ and

$$\phi_j(x) = \sin\left(\sqrt{\lambda_j}x\right) + \int_0^x K(x,t)\sin\left(\sqrt{\lambda_j}t\right)\mathrm{d}t. \tag{6}$$

Here the Gel'fand-Levitan function $K(x,t)$ satisfies

$$K_{tt} - K_{xx} + q(x)K = 0, \tag{7}$$

see [2, 15]. Note that since $\phi_1(0) = 0$ we will have $K(x,0) = K_x(0,t) = 0$. Now apply the boundary condition at $x = 1$ in equation (3) so that equation (6) becomes after setting $x = 1$

$$\begin{aligned}\int_0^1 [K_x(1,t) + \beta_j K(1,t)]\sin\left(\sqrt{\lambda_j}t\right)\mathrm{d}t = \sqrt{\lambda_j}\cos\left(\sqrt{\lambda_j}\right)\\ + (\beta_j + K(1,1))\sin\left(\sqrt{\lambda_j}\right) =: f_j, \quad 1 \leqslant j \leqslant B.\end{aligned} \tag{8}$$

where $K(1,1) = \frac{1}{2}\int_0^1 q(s)\,\mathrm{d}s$.

We can also integrate this by parts to obtain equations for the pair $[K_x(1,t), K_t(1,t)]$

$$\begin{aligned}\int_0^1 K_x(1,t)\sin(\sqrt{\lambda_j}t)\,\mathrm{d}t - \frac{\beta_j}{\sqrt{\lambda_j}}\int_0^1 K_t(1,t)\cos(\sqrt{\lambda_j}t)\,\mathrm{d}t = f_j\\ + \frac{\beta_j}{\sqrt{\lambda_j}}K(1,1)\Big)\cos(\sqrt{\lambda_j}) =: g_j\end{aligned} \tag{9}$$

again for $1 \leqslant j \leqslant B$.

From the now computed values of $\{\beta_j\}$ for each β_j we obtain f_j and then must recover $K(1,t)$, $K_x(1,t)$ and hence the pair $\{K_x(1,t), K_t(1,t)\}$ from the integral equation (8). From this Cauchy data pair the recovery of q follows directly in a very stable way as in [15] which we now explain. Note that in the second formulation, (9), there was a differentiation step in computing $K_t(1,t)$ and thus this aspect of the inversion has a mild degree of ill-conditioning and may seem relatively insignificant against the main terms and also benign in the sense that it would have to be paid regardless for the case of just using $K(1,t)$ and $K_x(1,t)$ as these would only have delivered the values $\int_0^x q(s)\,\mathrm{d}s$. In figure 1 to be shown below we see that the overall condition number of our key inversion matrix M does show a potentially significant difference, at least when involving the higher singular values.

Note that since $K(x,t) = -K(x,-t)$ for all x,t then both $K(1,t)$ and $K_x(1,t)$ will be odd functions about $t = 0$ and $K_t(1,t)$ will be an even function about $t = 0$ in the representations (8), (9). We thus should expand $K_x(1,t)$ as a sine series $\sum_1^N a_j\sin(j\pi t)$ and $K(1,t)$ also as a sine series $\sum_1^N b_j\sin(j\pi t)$, but $K_t(1,t)$ as a cosine series $\sum_0^N c_j\cos(j\pi t)$. Note also that c_0 need not be zero.

The simplistic approach is to use the Gel'fand-Levitan representation again mapping solutions of $q = 0$ onto the reconstructed q. In the 'usual cases' the terms in $\sqrt{\lambda_n}$ has $\lambda_n \approx n^2\pi^2$ and so $\{\sin\sqrt{\lambda_n}t\}$ is an almost orthogonal set. This will be far from true in the current situation and a value of $\beta = 100$ will be essentially Dirichlet conditions and with $\beta = 10$ a close approximation. The action will take pl ace in the region $\beta \in [0,10]$ and the most likely case is they should be more densely concentrated near zero. The approach we describe is based on [15].

Note that $K(1,0) = K_x(1,0) = 0$ and both $K(1,t)$ and $K_x(1,t)$ are odd. Hence we may represent $g(t) := K(1,t)$, $g_t(t) := K_t(1,t)$ and $g_x(t) := K_x(1,t)$ as the Fourier approximations

$$K(1,t) = \tfrac{1}{2}\bar{q}\,t + \sum_{j=1}^{N} a_j \sin(j\pi t), \quad K_t(1,t) = \sum_{j=0}^{N} c_j \cos(j\pi t),$$
$$K_x(1,t) = \sum_{j=1}^{N} b_j \sin(j\pi t) \tag{10}$$

where $\bar{q} = \int_0^1 q(x)\,dx$. An additional term such as $\frac{1}{2}\bar{q}t$ is needed since $K(x,x) = \frac{1}{2}\int_0^x q(s)\,ds$ and hence we must have $K(1,1) = \frac{1}{2}\bar{q}$. On the other hand $K(x,0) = 0$ for all $x \in [0,1]$ so we require $K(1,0) = 0$. Now set $a_0 = \frac{1}{2}\bar{q}$ and $b_0 = 0$ and seek to recover the pair $\{a_j\}_{j=0}^N$, $\{b_j\}_{j=1}^N$—meaning we have $2N+1$ unknowns. This will require measuring the lowest eigenvalue $\lambda(\beta) = \lambda_j$ for B values of β where $B \geqslant 2N+1$. This is totally consistent in terms of operation count with the two-spectrum or single spectrum/norming constant formulations: in general one needs N eigenvalue/parameter *pairs* to recover the first N Fourier modes of q.

A few remarks on the above are in order. First, it is not of course a requirement to use a Fourier basis for q here and there are certainly other options, but choosing a mutually orthogonal one will aid in minimising the condition number of the inversion process. Second, in the two-spectrum formulation where there are different boundary conditions for each spectral sequence the behaviour of their asymptotic values obey a well-structured formula. This means that for Dirichlet conditions on (0, 1) we have the asymptotic form $\lambda_n = n^2\pi^2 + \bar{q} + o(n^{-s})$ for $s > 0$ and for Dirichlet-Neumann conditions $\lambda_n = (n - \frac{1}{2})^2\pi^2 + \bar{q} + o(n^{-s})$ where the index s depends on the smoothness of the potential q, [15]. In particular, from this one can get a very good estimate of the mean $\bar{q}$ just from the data. This will *not* be the situation in our multi-impedance version as the range of spectral values will lie in the range $[\frac{\pi}{2}, \pi]$ translated by $\bar{q}$ for the lowest frequency case and so $\bar{q}$ has to be considered as an unknown to be itself determined. This requires at least one additional spectral measurement λ_j over the number N of basis functions to be used.

When we put the above together we have from (8) and (10) a matrix equation to solve for the Fourier coefficients. We examine only the case for recovering the pair $[K_t(1,t), K_x(1,t)]$ as the other case is completely analogous

$$\sum_{n=0}^{N} A_{jn} b_n + C_{jn} c_n = g_j, \quad b_0 = 0 \qquad \text{where}$$
$$A_{j,n} = \int_0^1 \sin\left(\sqrt{\lambda_j}\,t\right) \sin(n\pi t)\,dt, \qquad C_{j,n} = \int_0^1 \cos\left(\sqrt{\lambda_j}\,t\right) \cos(n\pi t)\,dt, \quad j = 1, \ldots, B. \tag{11}$$

Equation (11) can be written as the block matrix formulation

$$\sum_{n=0}^{2N} \mathbf{M}_{jn} c_n = g_j \qquad \text{where } \mathbf{M}_{jn} = \begin{pmatrix} A_{jn} & \tilde{\beta}_j C_{jn} \end{pmatrix}, \quad \tilde{\beta}_j = -\frac{\beta_j}{\sqrt{\lambda_j}}, \quad c_n = \begin{pmatrix} b_n \\ c_n \end{pmatrix} \tag{12}$$

where $\mathbf{M}$ is a $B \times 2N+1$ matrix and $\{c_n\}$ a $2N+1$ vector.

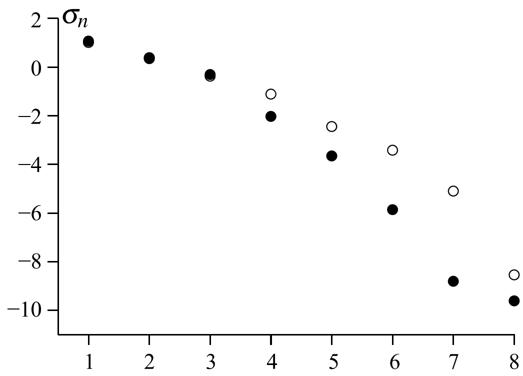

Figure 1. Singular values σ_n of M.

What is important here is to compute the singular values for the matrix **M** to see how these depend on the values of the impedance $\{\beta_j\}$ to determine the optimal choices for these in order to minimise the condition number of **M**. In fact, this is far from necessary in a precise way; the key is to have as large a range as possible on $(0,\infty)$, that is between Dirichlet and Neumann conditions and to have a spread. In practice we computed B equal values not in β but in λ_0 corresponding to $q=0$; that is between $\frac{\pi^2}{4}$ and π^2. For each such λ_0 we then computed the corresponding endpoint impedance value β. Note that the range of $\sqrt{\lambda}$ will be a small perturbation of the mean of $q(x)$ plus the $[\frac{\pi^2}{4},\pi^2]$ so that $\sqrt{\lambda}$ will have range roughly $\sqrt{\bar{q}}+[\frac{\pi}{2},\pi]$.

Figure 1 shows the first several singular value of the matrix M in equation (12) for the case of the zero potential. These were computed using ten values of β chosen so that the resulting $\lambda(\beta)$ were approximately evenly spaced between $(n+\frac{1}{2})\pi$ and $(n+1)\pi$ for the potential $q=0$ when $\beta\in[0,100]$.

We show only the singular values of the matrix M in (12) formed from computing the lowest value spectrum: that is the smallest eigenvalue for each β as this is the basic paradigm of feasible measurements. There are two sequences, one from recovering the pair $[K_t(1,t),K_x(1,t)]$ corresponding to equation (8) (using the symbol $\circ$) and the other from (9) to recover $[K(1,t),K_x(1,t)]$ (using the symbol $\bullet$). We show both to illustrate the subtle point noted above: recovering the former pair is slightly less ill-conditioned than for the latter pair. This coupled with the fact that we do not need a further differentiation to recover $q(x)$ in the second case but do in the first as will be seen in the next section.

Several things that were expected now become immediately clear. First, each of the individual singular value sequences coming from using the first, second, third, etc eigenvalue set as the impedance parameter β was varied, decay exponentially to zero. Second, if only the lowest eigenvalue was used for each β then under anything but extremely accurate data no more than the first 5 or 6 singular values can be used. In this situation, which as we have seen includes the parabolic equation case, shows that only quite limited frequency information about the potential q can be extracted. The subdiffusion model to be considered in section 7 with its only linear time-decay is able to utilise more of the singular values to advantage in the recovery of q. Third, many more usable singular values become available for use when further eigenvalue sets are included: we will see this clearly in figure 4 shown in section 7. The above is to be expected as we know that excellent reconstructions, especially for a relatively smooth q, can be obtained from a modest number of eigenvalue measurements for each of just two impedance values, that is, the two spectrum formulation of Borg. See [15] for examples of such reconstructions.

5. Recovering $q(x)$ from the Cauchy values K, K_x

The geometric configuration and conditions on the kernels $K(x,t)$ are shown in the figure 2 below.

If $q(x)$ is known then we have a hyperbolic equation with Goursat data $\int_0^x q(s)\,ds$ and can thus recover $K(x,t)$ within the shaded triangle and in particular obtain the Cauchy values $K(1,t)$ and $K_x(1,t)$. Note that since $K(x,0)=0$ we can reflect the Cauchy data as odd functions for $t<0$.

Alternatively, we can take a function $q(x)$ and use the Cauchy values at $x=1$ to find $K(x,t)$ within the triangle. Of course, there is no reason to expect that the obtained values at $x=t$ will correspond to $\int_0^x q(s)\,ds$. To achieve this requires an iterative process to be described below.

We can just consider the region $t\geq 0$ and use the known value $K(x,0)=0$ as a boundary condition for the hyperbolic equation. This is more efficient if, for example, a finite difference scheme is used.

There are two approaches to recovering $q(x)$ from the data pair $\{g(t), g_x(t)\}$ derived from the values $\{K(1,t), K_x(1,t)\}$. The first is to solve the map $q \mapsto \{\frac{g(t)}{g_x(t)}\}$ by, for example, Newton's method making an initial approximation q_0 for q. This in fact converges quite rapidly even for large $q(x)$ but requires computing the Goursat data $\int_0^x q(s)\,ds$ by quadrature at each iteration. A simpler version is to use a 'quasi-Newton' method obtained by computing the derivative of the map frozen at $q=0$. In this situation we have things in closed form and local injectivity of the derivative map follows immediately.

The second method is to use successive approximations by solving a Cauchy problem with data values $K(1,t)=g(t)$, $K_x(1,t)=g_x(t)$. One reason this works is due to the approximations

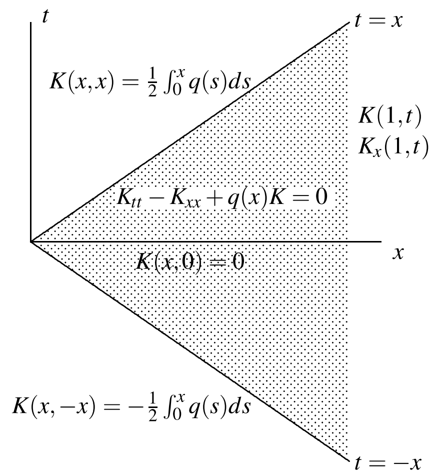

Figure 2. $K(x, t)$ function.

$$\frac{1}{2}\left[q((x+t)/2)+q((x-t)/2)\right]\approx K_t(1,t) \qquad \frac{1}{2}\left[q((x+t)/2)-q((x-t)/2)\right]\approx K_x(1,t). \tag{13}$$

Again, one needs an initial approximation q_0 for the hyperbolic equation and this can be obtained from the above. The update is obtained from

$$q_{n+1}(x)=2\frac{\mathrm{d}}{\mathrm{d}x}K(x,x;q_n). \tag{14}$$

Convergence here is also extremely rapid; typically 4 or 5 iterations suffice.

An alternative formulation of this scheme is to define $v=v(x,t;q)$ by

$$v_{tt}-v_{xx}+q(x)v=0, \qquad v(x,0)=0, \qquad v(x,x)=\frac{1}{2}\int_0^x q(s)\,\mathrm{d}s \tag{15}$$

then recover $q(x)$ by the iterative scheme.

$$q_{n+1}=q_n(x)+2\big(K_t(1,2x-1)+K_x(2x-1)\big)-v_t(1,2x-1)-v_x(1,2x-1). \tag{16}$$

For the analysis and convergence proofs for these methods and statements see [15].

Remark 5.1. The main reason for bringing both $K(1,t)$ and $K_t(1,t)$ into the discussion earlier is now apparent: in one case this is the natural situation for equation (13) and in the other for equation (14).

6. A reconstruction example

As noted previously, our model has normalised the combined diffusion coefficient coupling the time and spatial scales to unity and an inverse scaling is then required to recover actual time. Under this paradigm $t=1$ corresponds to a very large physical time.

We are assuming that the variable boundary condition is at the right hand endpoint $x=1$ and we are free to fix the boundary condition at $x=0$. If our goal is minimise the eigenvalues to lessen the solution decay then taking Neumann conditions at $x=0$ is optimal and Dirichlet conditions give the largest λ. This choice may not be available for a specific application.

In practice we selected the parameters $\{\beta_i\}$ by the following process. For $q=0$ the lowest eigenvalues on $[0,1]$ range from 0 to $\frac{\pi}{2}$ in the case of Neumann conditions $u_x(0,t)=0$ and from $\frac{\pi}{2}$ to π in the case of Dirichlet conditions $u(0,t)=0$. In each case we took equally spaced eigenvalues for $q=0$ and then computed the corresponding $\{\beta_i\}_{i=1}^{B}$ in order to better capture the growth characteristics of what is an arctangent function in the case of $q=0$.

Data was formed using by a Crank-Nicolson solver and values $f(t)=u(1,t;\beta)$ obtained as our experimental time trace information. In the case of the fractional subdiffusion model of the next section a similar time stepping method was used. We set the grid so that the estimated error in $f(t)$ was approximately 0.5%. We then took a sample of S time values in $[T,T+L]$ of $f(t)$ for each β. In the graphic to be shown the values $T=1$, $L=\frac{1}{10}$, $B=21$ and $S=5$ was used for a total of BS data points.

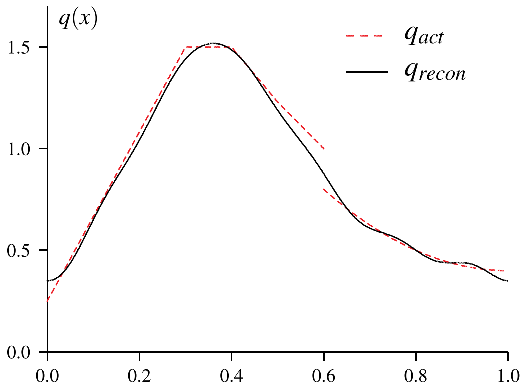

Figure 3. Reconstruction of $q(x)$.

The eigenvalues $\{\lambda_n\}$ were then estimated by the process described in section 3 and in turn these were used to reconstruct the values $K_t(1,t;q)$ and $K_x(1,t;q)$ as in section 4. The inversion of the matrix M introduced there can be accomplished using either truncated svd or adding a Tikhonov regularising term. In producing the figure below we used the latter approach.

In figure 3 we show a reconstruction of a piecewise continuous function $q(x)$ with a discontinuity near the midpoint, is not differentiable at several places and not periodic but it lies in $L^2(0,1)$. A Fourier basis was used for $K_t(1,t)$ and $K_x(1,t)$ as noted previously and we also used a Fourier basis to represent $q(x)$. The initial approximation $q_0 = 0$ was taken and q recovered by equation (16). Effective convergence was obtained after 4 or 5 iteration and this was typically the case over a broad range of phantoms $q(x)$.

Since we used a Fourier basis to represent $q(x)$ this will yield a reconstructed $q(x)$ with periodicity imposed. Thus the sharp edges/discontinuity in the graph could not be resolved completely and the endpoint values are incorrect. Of course, if we have prior knowledge of the function q then alternative basis functions would be appropriate. The important point though is the fact that we are able to achieve a good fit within this standard chosen basis and thus taking a non-orthogonal basis is likely to increase the condition number of the matrix M and hence result in overall poorer reconstructions due to the increased regularisation that will be needed. The trade-off involved could be delicate here.

7. Other models

In a time-dependent situation where the experimental set up allows the change of boundary conditions the paradigm described in the last sections has applicability to extend the range of existing inverse problem models. In this section we look at two such possible cases where we replace the parabolic equation in (1) by two models of time-dependent situations: a subdiffusion operator where the time derivative is based on an Abel fractional operator of Djrbashian type and a damped, possibly nonlinear, wave equation. In each case we make the assumption that our unknown coefficient is spatially dependent, we have the ability to change the boundary conditions and our measurement data consists of a time-trace which is only available for large time values. For background information on these models see [5, 8, 16, 17] or the book [7].

The fractional subdiffusion equation of order α we consider is the generalisation of the parabolic

$$
\begin{aligned}
&\partial_t^\alpha - \triangle u + q(x)\,u = 0, \\
&Bu = \frac{\partial u(x,t)}{\partial \nu} + \beta u = 0 \qquad x \in \partial\Omega, \quad t > 0, \\
&u(x,0) = u_0(x) \qquad x \in \Omega.
\end{aligned} \tag{17}
$$

The solution representation for (17) becomes

$$
u(x,t) = \sum_1^\infty a_n E_\alpha\left(-\lambda_n t^\alpha\right)\phi_n(x). \tag{18}
$$

where $E_\alpha(z)$ is the Mittag–Leffler function of order α, $0<\alpha<1$. The fundamental difference is that the large time behaviour is now governed by the asymptotics of $E_\alpha(z)$ with the result that the solution decays only linearly in t^α. This means that the severe ill-conditioning arising from the exponential function decay is now replaced by a linear decay.

$$
E_\alpha\left(-\tau\right) = \sum_{k=0}^{N} \frac{1}{\Gamma\left(1-\alpha k\right)}\frac{1}{\tau^k} + O\left\{\frac{1}{t^{N+1}}\right\} \quad \text{with } \tau = t^\alpha. \tag{19}
$$

Thus the problem is still ill-posed but to a significantly milder degree. See, for example, [5, 7]. On the other hand, benefit from using multiple experiments with a changing β parameter is still relevant.

We remark that such fractional models have been proposed as regularising operators for time-reversal questions such as the classical backwards heat problem, [7, 17, 19]. Central to this is the fact that as $\alpha \to 1$ the Mittag–Leffler function with negative argument is continuous from below and converges to the exponential function, [7]. It thus makes an appropriate choice for such quasi-reversibility techniques. See for example, [5–7, 18, 19].

However, the likelihood is that for sufficiently large T values and for larger eigenvalue indices (that is n represents the k^{th} eigenvalue corresponding to a given β) the values of the solution are sufficiently small to lie outwith our error tolerances. This will again limit the maximum usable indices for λ_n. Thus, for each impedance parameter β we may obtain the spectrum $\lambda_{k,\beta}$ for all β but k in the range $1 \leqslant k \leqslant k_{\max}$. Clearly, this is now overposed information but it will help in reducing the condition number of the matrix M in (12). Figure 4 confirms this statement. It shows the singular values of M when the first ($M^{(1)}_\lambda$), first and second ($M^{(2)}_\lambda$) and first three ($M^{(3)}_\lambda$) eigenvalues of the β-sequence are all used. The resulting reduction in the condition number can be substantial.

As a second example of a model fitting the framework of being recovered from only large time measurements is the damped wave equation $u_{tt} - a(x)u_{xx} + du_t = 0$ with initial values $u_0(x)$ and $u_{t0}(x)$ and boundary conditions $u(0,t) = 0$, $u_x(1,t) + \beta u(1,t) = 0$. This has sinusoidal solutions that decay exponentially with rate proportional to d. Thus for large time values we are in exactly the same situation as with the heat equation: the recovery of the eigenvalues of the operator $a(x)u_{xx} = -\lambda_n u$ from time trace data will be an extremely ill-conditioned problem. The likelihood is that once again only the lowest spectral values, $k = 1$ for each impedance value β would likely be available from the time series.

Certain nonlinear wave equations can also be treated with this approach. An example is the damped Westervelt equation which is the basis of modelling ultrasound in a lossy media. This

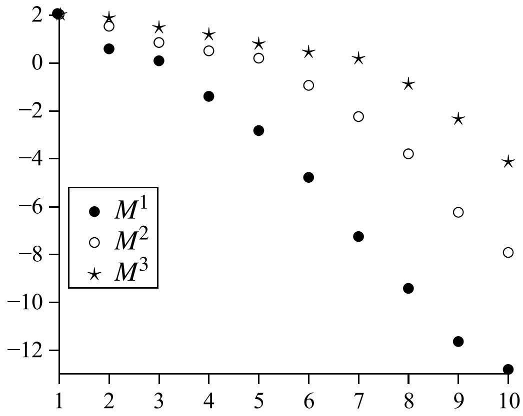

Figure 4. Singular values of $\{M^i\}_{i=1}^3$.

amounts to identification of the space dependent coefficient $\kappa(x)$ for the attenuated Westervelt equation in pressure formulation. In a single spatial variable this is

$$\begin{cases} \left(v-\kappa(x)v^2\right)_{tt} - c(x)^2 v_{xx} + \mathscr{D}v = 0 \quad \text{in} \quad [0,1]\times(0,T) \\ v_x(0,t) = v_x(1,t) = 0 \\ v(x,0) = v_0(x), \quad v_t(x,0) = v_1(x), \quad x\in(0,1) \end{cases} \tag{20}$$

where $c(x)$ is the wave speed at position x and $\mathscr{D}$ is a damping term which we take to be of the form $\mathscr{D}u = du_t$.

The solutions of (20) also decay exponentially in time. This means that with our assumption of only large time values the nonlinear term $\kappa(x)v^2$ becomes negligible against v and now for all practical purposes our model reduces to a damped wave equation with again possibly unknown wave speed $c(x)$. In this situation $c(x)$ can be recovered from such time measurements as in the linear case above.

Now if we had time trace measurements for all times (or just for very short and very large t values) then this would lead to a decoupling of the two unknown coefficients. The large time values would be used to obtain $c(x)$ and then with this known, small time values could be used to recover $\kappa(x)$. This approach, but using Newton's method to solve the resulting nonlinear equations, was taken in [8].

We also remark that the damping term $\mathscr{D}$ is often taken to be of fractional type; for example, at the simplest level $\mathscr{D}u = dD_t^\alpha u$. This results in a slower decay of the solution in time in an entirely analogous way to the subdiffusion situation. For further information here we refer to the book [7].

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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