# **Recovery of a potential in a fractional diffusion equation**

William Rundell\*

Masahiro Yamamoto<sup>†</sup>

November 15, 2018

#### Abstract

We consider the determination of an unknown potential q(x) form a fractional diffusion equation subject to overposed lateral boundary data. We show that this data allows recovery of two spectral sequences for the associated inverse Sturm-Liouville problem and these are sufficient to apply standard uniqueness results for this case.

We also look at reconstruction methods and in particular examine the issue of stability of the solution with respect to the data. The outcome shows the inverse problem to be severely ill-conditioned and we consider the differences between the cases of fractional and of classical diffusion.

#### 1 Introduction

A standard inverse problem is to recover a coefficient in an elliptic operator  $\mathbb{L}$  from the diffusion equation  $u_t + \mathbb{L}u = 0$  from a combination of initial data  $u_0(x) = u(x,0)$  and over-specified boundary data. For example, with  $\mathbb{L} = -u_{xx} + q(x)u$  on the domain  $(0,1) \times (0,T)$  we might impose homogeneous boundary conditions, say the flux,  $u_x(0,t) = u_x(1,t)$  and measure the data u(0,t) = g(t) from which we would hope to recover q(x) for a given initial value  $u_0(x)$ . Of course, we might also reverse the type of the boundary conditions. Another possibility is to choose homogeneous initial conditions  $u_0(x) = 0$ and lateral conditions at x = 0, u(0,t) = 0, but now impose Cauchy data on the other lateral boundary x = 1.

Some of these approaches were taken in [12] for the case of the parabolic operator, but we are also interested in the subdiffusion model involving fractional derivatives and extending the parabolic case to one of a subdiffusion process using a Djrbashian-Caputo fractional derivative with index  $\alpha$ ,  $0 < \alpha \leq 1$ . Fractional diffusion equations with Caputo derivatives in time have been widely used as model equations for describing the anomalous diffusion phenomena. Two important cases are highly heterogeneous aquifers and complex viscoelastic material; see [1, 6] and also [16] for further applications.

As a by-product of the analysis we will expand upon known results for the parabolic case  $\alpha = 1$ . The primary goal of this paper is to establish uniqueness results, but we will also compare the degree of ill-conditioning of the problem with respect to  $\alpha$ . The latter is also of physical interest as it indicates whether model reconstruction problems for the fractional case differ substantially from the classical. The now classical example of the backwards diffusion problem for both the classical and fractional cases illustrates this possibility where the degree of ill-conditioning differs remarkably [10, 15]. However, depending on the value of the final time *T* this may not translate into a superior numerical recovery for the backwards fractional case  $\alpha < 1$ , as shown in [8, 9].

<sup>\*</sup>Department of Mathematics, Texas A&M University, College Station, Texas 77843 USA. rundell@math.tamu.edu <sup>†</sup>Department of Mathematical Sciences, The University of Tokyo, Tokyo 153 Japan. myama@ms.u-tokyo.ac.jp

Specifically, we shall consider the following problem; suppose u(x,t) satisfies

Here  ${}_{0}^{C}D_{t}^{\alpha}$  denotes the Djrbashian-Caputo fractional derivative of order  $\alpha$ ,  $0 < \alpha \leq 1$ , with starting point the left-hand boundary x = 0. The potential q(x) is assumed to be unknown and in order to utilize existing results for 1, we take  $q(x) \in L^{\infty}$  although weaker conditions, for example  $q \in L^{2}$  would suffice if we only consider the question of uniqueness. We also might impose a nontrivial value of  $u_{0}(x) = u(x,0)$ . However, regularity of the direct problem, namely given q(x) determine u(x,t), becomes a delicate issue in terms of the smoothness imposed on  $u_{0}(x)$  and we prefer to avoid issues that are tangential to the main theme. We remark that in general the fractional order operator in 1 has limited smoothing properties and this, together with the nonhomogeneous version, 8 to be considered below, is such that the solution u has regularity that depends strongly on the initial data, [15].

The current work also has ideas in common with [4] where the unknown coefficient appeared in the operator as a diffusion coefficient a(x),  $\mathbb{L}u := (a(x)u_x)$  although in this work the boundary conditions were homogeneous and the initial data was  $u_0(x) = \delta(x)$ . If in the current situation we had instead the operator taken this operator then the inverse Sturm-Liouville uniqueness will still go through but the analysis of reconstruction would require modifications.

Under the above conditions, there is a unique solution to 1 for any sufficiently smooth a(t) and any  $\alpha$ ,  $0 < \alpha \le 1$ , see [15].

For reasons that will become apparent we shall restrict a(t) to be integrable and have compact support on the interval [0, T] for some fixed T > 0.

Our goal is in addition to measure the flux data

$$u_x(1,t) = b(t), \qquad t > T \tag{2}$$

and from the pair  $\{a(t), b(t)\}$  seek to determine the unknown potential q(x).

## 2 Background for fractional operators

An essential component of fractional derivative problems is the two-parameter Mittag-Leffler function  $E_{\alpha,\beta}(z)$  defined by

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)} \quad z \in \mathbb{C},$$
(3)

for  $\alpha > 0$ , and  $\beta \in \mathbb{R}$ . This generalizes the exponential function ubiquitous to classical diffusion;  $E_{1,1}(z) = e^{z}$ .

**Lemma 2.1** For any  $\alpha > 0$  and  $\beta \in \mathbb{R}$ ,  $E_{\alpha,\beta}(z)$  is an entire function of order  $\frac{1}{\alpha}$  and type 1.

**Lemma 2.2** *For*  $0 < \alpha \le 1$  *and* x > 0,  $\lambda > 0$ 

$$\alpha \lambda \frac{d}{dx} E_{\alpha,1}(-\lambda x) = -E_{\alpha,\alpha}(-\lambda x) \tag{4}$$

*For*  $\operatorname{Re}(\alpha) > 0$  *and*  $\operatorname{Re}(\beta) > 1$  *and from*  $\lambda$  *real* 

$$\frac{d}{dx}x^{\beta-1}E_{\alpha,\beta}(\lambda x^{\alpha}) = x^{\beta-2}E_{\alpha,\beta-1}(\lambda x^{\alpha})$$
(5)

*For*  $\Re(\alpha) > 0$  *and*  $\Re(\beta) > 0$  *and a real* 

$$\frac{d}{dz}E_{\alpha,\beta}(az) = \frac{a}{\alpha z} \left( E_{\alpha,\beta-1}(az) - (\beta-1)E_{\alpha,\beta}(az) \right)$$
(6)

**Lemma 2.3** Let  $\alpha \in (0,1]$ ,  $\beta \in \mathbb{R}$ ,  $z \ge 0$ , and  $N \in \mathbb{N}$ . Then with  $z \to \infty$ ,

$$E_{\alpha,\beta}(-z) = \sum_{k=1}^{N} \frac{(-1)^{k-1}}{\Gamma(\beta - \alpha k)} \frac{1}{z^k} + O\left(\frac{1}{z^{N+1}}\right).$$
(7)

Following standard practice we transform equations 1 into a set with homogeneous boundary conditions using v(x,t) = u(x,t) - a(t) to obtain

$$D_t^{\alpha} v(x,t) - v_{xx}(x,t) + q(x)v(x,t) = f(x,t), \qquad 0 < x < 1, \quad t > 0$$
  

$$v_x(0,t) = 0, \quad v_x(1,t) = 0, \quad t > 0$$
  

$$v(x,0) = 0, \quad 0 \le x \le 1$$
(8)

with  $f(x,t) = -(D_t^{\alpha}a(t) + q(x)a(t)).$ 

We assume that  $D_t^{\alpha}a(t) \in L^{\infty}(0,T)$ . With  $\Omega = (0,1)$ , then  $f \in L^2(\Omega \times (0,t^*))$  for any fixed  $t^*$  and there exists a unique weak solution  $v(x,t) \in L^2(0,t^*;H^2(\Omega) \cap H_0^1(\Omega))$  such that

$$\|u\|_{L^{2}(0,t^{*}),H^{2}(\Omega)} + D_{t}^{\alpha} u\|_{L^{2}(0,t^{*}),L^{2}(\Omega)} \le C \|f\|_{L^{2}(\Omega) \times (0,t^{*}))}$$
(9)

See [15, Theorem 2.2].

The solution to 8 is easily obtained by separation of variables. Let  $\{\lambda_j, \phi_j(x;q,\lambda_j)\}_1^\infty$  be the Neumann eigenvalues and eigenfunctions of  $-\phi_j'' + q\phi_j = \lambda_j\phi_j$ , that is, with  $\phi_j'(0) = \phi_j(1) = 0$ . Let  $\{\tilde{\phi}(x)\}$  denote the eigenfunctions with the normalization  $\|\phi\|_L^2 = 1$ . Then from [8, 15] the solution to 8 is given by

$$v(x,t) = \sum_{j=1}^{\infty} \int_0^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}(-\lambda_j(t-\tau)^{\alpha}) \langle f(\cdot,\tau), \,\tilde{\phi}_j \rangle \, d\tau \, \tilde{\phi}_j(x). \tag{10}$$

However, it will be more convenient for our purposes to assume an endpoint normalization, more typical of Sturm-Liouville theory and therefore we will instead use the normalization  $\phi(1) = 1$  in place of  $\|\phi\|_{L^{2}}^{2} = 1$ . Under this assumption we then set  $\rho_{j} = \|\phi\|_{L^{2}}^{2}$ . Also, without loss of generality, we may assume  $\lambda_{j} > 0$ , for  $j \in \mathbb{N}$ .

From 10 we now obtain for the original dependent variable evaluated at the right-hand boundary

$$u(1,t) = \sum_{j=1}^{\infty} \rho_j \int_0^t s^{\alpha-1} E_{\alpha,\alpha}(-\lambda_j s^\alpha) a(t-s) ds, \quad 0 < t < T.$$

$$\tag{11}$$

An integration by parts using the assumption a(0) = 0 yields

$$\int_0^t s^{\alpha-1} E_{\alpha,\alpha}(-\lambda_j s^{\alpha}) a(t-s) ds = -\frac{1}{\lambda_j} \int_0^t \frac{d}{ds} (E_{\alpha,1}(-\lambda_j s^{\alpha})) a(t-s) ds$$

$$= -\frac{1}{\lambda_j} a(t) - \frac{1}{\lambda_j} \int_0^t E_{\alpha,1}(-\lambda s^{\alpha}) a'(t-s) ds,$$
(12)

and so

$$u(1,t) = -\sum_{j=1}^{\infty} \frac{\rho_j}{\lambda_j} a(t) - \sum_{j=1}^{\infty} \frac{\rho_j}{\lambda_j} \int_0^t E_{\alpha,1}(-\lambda_j s^\alpha) a'(t-s) \, ds \quad 0 < t < T.$$
(13)

We know that  $\rho_n = c_0 + o(1)$  as  $n \to \infty$ , [13], and so

$$\sum_{j=1}^{\infty} \left| \frac{\rho_j}{\lambda_j} \right| < \infty.$$

Therefore, setting

$$b = -\sum_{j=1}^{\infty} \frac{\rho_j}{\lambda_j}, \quad A(t) = \sum_{j=1}^{\infty} \frac{\rho_j}{\lambda_j} E_{\alpha,1}(-\lambda_j t^{\alpha}),$$

we obtain  $b < \infty$  and  $A \in C[0, \infty)$ . We can rewrite 13 as

$$u(1,t) = -ba(t) - \int_0^t A(s)a'(t-s)ds = \int_0^t (-b - A(s))a'(t-s)ds, \quad 0 < t < T$$
(14)

since a(0) = 0, this implies  $a(t) = \int_0^t a'(t-s) ds$ .

Now let  $\sigma_n = \|\psi_n\|_{L^2(0,1)}^{-2}$  and set  $c = -\sum_{j=1}^{\infty} \frac{\sigma_j}{\mu_j}$  and  $B(s) = \sum_{j=1}^{\infty} \frac{\sigma_j}{\mu_j} E_{\alpha,1}(-\mu_j s^{\alpha})$ . Since u(p)(1,t) = u(q)(1,t), 0 < t < T, we have

$$\int_0^t (b + A(s))a'(t - s) \, ds = \int_0^t (c + B(s))a'(t - s) \, ds, \quad 0 < t < T.$$

Titchmarsh's theorem and the analyticity in t of A and B for  $\operatorname{Re} t > 0$  yields

$$b + A(t) = c + B(t), \quad 0 < t < \infty.$$

Taking the Laplace transform then implies

$$\frac{b}{z} + \sum_{j=1}^{\infty} \frac{\rho_j}{\lambda} \frac{z^{\alpha-1}}{z^{\alpha} + \lambda} = \frac{c}{z} + \sum_{j=1}^{\infty} \frac{\sigma_j}{\mu_j} \frac{z^{\alpha-1}}{z^{\alpha} + \mu_j}$$

for Re z > 0. Multiplying with  $z^{1-\alpha}$  and setting  $\eta = z^{\alpha}$ , we obtain

$$\frac{b}{\eta} + \sum_{j=1}^{\infty} \frac{\rho_j}{\lambda} \frac{1}{\eta + \lambda} = \frac{c}{\eta} + \sum_{j=1}^{\infty} \frac{\sigma_j}{\mu_j} \frac{1}{\eta + \mu_j}$$
(15)

for Re  $\eta > 0$ . By analyticity with respect to  $\eta$  we see that the two representations in 15 must agree and so both the pole locations and their residues must be identical. This gives

$$b = c$$
,  $\lambda_i = \mu_i$ ,  $\rho_i = \sigma_i$ , for all  $j \in \mathbf{N}$ .

The Gel'fand-Levitan theory for the potential-form inverse Sturm-Liouville problem will now yield the uniqueness result

**Theorem 2.1** Suppose that a(t) has support on the interval [0,T] and that  $D_t^{\alpha}a(t) \in L^{\infty}[0,T]$ . Then there is at most one solution  $\{q(x), u(x,t)\}$  to 1 and 2.

Since we will need this construction for the computational examples the proof of this fact and its relation to 1 will now be briefly presented.

#### 3 The inverse Sturm-Liouville problem

We denote by  $\phi(x;q,\lambda)$  the solution of

$$-\phi''(x) + q(x)\phi(x) = \lambda\phi(x), \qquad \phi(0) = 0, \quad \phi'(0) = 1.$$
(16)

For each q there is clearly a unique solution  $\phi(x)$  to 16. We will impose boundary conditions at x = 1 and look for the associated eigenvalue/eigenvector pairs  $\{\lambda_n, \phi_n(x)\}_{n=1}^{\infty}$  and so we should view the condition  $\phi'(0) = 1$  as being a normalization of the eigenfunctions.

**Lemma 3.1** Let  $q_1$  and  $q_2 \in L^2(0,1)$  be two potentials. Suppose we are given that the Dirichlet eigenvalues  $\{\lambda_n\}$  of 16 for each of  $q_1$  and  $q_2$  are identical; that is  $\phi_n(1;q_1,\lambda_n) = \phi_n(1;q_2,\lambda_n) = 0$ . If further, the eigenvalues  $\{\mu_n\}$  for the case of Neumann boundary conditions at x = 1 are also identical; that is  $\phi'_n(1;q_1,\mu_n) = \phi'_n(1;q_2,\mu_n) = 0$ , then  $q_1 = q_2$  a.e.

Lemma 3.1 is the famous two spectrum result of Borg, [2]. Since the original paper there have been several proofs of this result and we will outline one below since the underlying machinery will be needed in a later section.

The Gel'fand-Levitan transformation maps solutions of 16 with  $q = q_1$  into solutions with  $q = q_2$ and is given by

$$\phi(x;q_2,\lambda) = \phi(x;q_2,\lambda) + \int_0^x K(x,t)\phi(t;q_1,\lambda)\,dt \tag{17}$$

where K(x,t) is independent of  $\lambda$  satisfies the hyperbolic equation

$$K_{tt} - K_{xx} + (q_1(x) - q_2(t))K = 0, \qquad 0 < t \le x \le 1$$
  

$$K(x, \pm x) = \pm \frac{1}{2} \int_0^x [q_2(s) - q_1(s)] ds, \quad K(x, 0) = 0, \qquad 0 \le x \le 1.$$
(18)

For a proof of this computation see, [13] or the original paper, [5].

Now suppose  $\phi_n(1;q_1,\lambda_n) = \phi_n(1;q_2,\lambda_n)$  for each positive integer *n*. Then from 17 it follows that  $\int_0^1 K(1,t)\phi(t;q_1,\lambda_n) dt = 0$  and from the completeness of the Dirichlet eigenfunctions that K(1,t) = 0. If now  $\phi'_n(1;q_1,\mu_n) = \phi'_n(1;q_2,\mu_n)$  then in a similar manner we obtain  $K_x(1,t) = 0$ . Under these conditions K(x,t) satisfies a homogeneous hyperbolic equation in the region  $\{(x,t): 0 \le t \le x \le 1\}$  with zero Cauchy data on the line x = 1. It must therefore be identically zero in this region and hence also on the boundary line x = t, that is, K(x,x) = 0. From the second equation in 18 we immediately obtain  $q_1 = q_2$  a.e. This proof was first shown in [17] and used as the basis for solving other inverse Sturm-Liouville problems in a constructive manner in [13].

Some of these other inverse spectral problems include replacing the second spectrum by an endpoint condition on the derivative at x = 1. That is, we are given the Dirichlet eigenvalues  $\{\lambda_n\}$  and together with the values of the derivative of the associated eigenfunctions at x = 1,  $\phi'(1;q,\lambda_n)$ . This is easily converted to the previous case. The common Dirichlet spectrum gives K(1,t) = 0 as before while the condition  $\phi'(1;q_1,\lambda_n) = \phi'(1;q_2,\lambda_n)$  when used in 17 immediately shows that  $K_x(1,t) = 0$ .

The original Gel'fand-Levitan paper showed uniqueness when the Dirichlet spectrum  $\{\lambda_n\}$  was given together with the norming constants  $\rho_n := \|\phi(x;q,\lambda_n)\|^2$ . With the above formulation we can easily convert endpoint problem data to norming constant data as follows (see [13]).

We can view equation 17 as mapping solutions of equation 16 with the zero potential onto that with potential q through

$$\phi(x;q,\lambda) = \phi(x;0,\lambda) + \int_0^x K(x,t)\phi(t;0,\lambda)\,dt = \frac{1}{\sqrt{\lambda}} \left[\sin(\sqrt{\lambda}) + \int_0^x K(x,t)\sin(\sqrt{\lambda})\,dt\right]$$
(19)

Then if we differentiate the equation  $-y'' + qy = \lambda y$  with respect to  $\lambda$  we obtain  $-\dot{y}'' + q\dot{y} = \lambda \dot{y} + y$ where  $\dot{y}$  denotes  $\frac{\partial y}{\partial \lambda}$ . Multiplying this by y, the original equation by  $\dot{y}$  and subtracting gives  $y^2 = y''\dot{y} - \dot{y}''y$ . Integrating between x = 0 and x = 1 and setting  $\lambda = \lambda_n$  (so y becomes  $\phi_n(x)$ ) we get

$$\int_0^1 \phi_n^2 dx = \dot{\phi}_n(1)\phi_n'(1)$$

and therefore

$$\rho_n = \dot{\phi}_n(1)\phi'_n(1) \quad \text{or} \quad \phi'_n(1) = \frac{\rho_n}{\dot{\phi}_n(1)}.$$
(20)

We ant to convert the data  $\{\rho_n\}$  into end-point data  $\{\phi'_n(1)\}$  and so we need an expression for  $\dot{\phi}_n(1)$ .

If we differentiate 19 in  $\lambda$  we obtain

$$\dot{\phi}(x) = -\frac{1}{2\lambda^{3/2}}\phi(x) + \frac{1}{2\lambda}\left\{\cos\sqrt{\lambda} + \int_0^1 tK(1,t)\cos\sqrt{\lambda}t\,dt\right\}.$$

Since  $\phi_n(1) = 0$  we get

$$\dot{\phi}_n(1) = \frac{1}{2\lambda} \left\{ \cos\sqrt{\lambda_n} + \int_0^1 t K(1,t) \cos\sqrt{\lambda_n} t \, dt \right\}$$

and so from 20 we obtain

$$\phi_n'(1) = \frac{2\lambda_n \rho_n}{\cos\sqrt{\lambda_n} + \int_0^1 t K(1,t) \cos\sqrt{\lambda_n} t \, dt}.$$
(21)

The Dirichlet spectrum  $\{\lambda_n\}$  gives K(1,t) as before and in 21 we immediately obtain  $\rho_n$  from  $\phi'_n(1)$ . We summarize this as follows,

**Lemma 3.2** Suppose we are given the Dirichlet spectra  $\{\lambda_n\}_1^{\infty}$  for a potential q and in addition, one of

1. For each spectral value  $\lambda_n$  we are given the endpoint derivative  $\phi'(1, q, \lambda_n)$ 

2. For each spectral value  $\lambda_n$  the  $L^2$  norm of the eigenfunction,  $\rho_n = \|\phi(1, q, \lambda_n)\|$ .

Then either  $\{\lambda_n, \phi'(1, q, \lambda_n)\}$  or  $\{\lambda_n, \rho_n\}$  uniquely determines q.

From the representation 21 we immediately obtain that

**Corollary 3.1** If we have the Dirichlet spectra  $\{\lambda_n\}_1^{\infty}$  and in addition the combination  $[\phi'(1)]^2 / \rho_n$  for each  $n \ge 1$ , then this determines q uniquely.

**Remark 3.1** We can also replace 2 by one measuring the flux on the leftmost boundary by using an almost identical analysis.

While aesthetically pleasing, the above analytic continuation-based proof should indicate the likelihood of the problem being severely ill-conditioned. The two spectrum version of the inverse Sturm-Liouville problem is only mildly ill-conditioned (although we will have some caveats to add to this later) and the problem is transitioning the data function b(t) into the precise location of the zeros and poles of its complex-valued Laplace transform. In the parabolic case we must locate the zeros and poles located on the negative real axis in *s*-space from values obtained by integrating the data b(t)against an exponentially decaying function to obtain  $\hat{b}(s)$  for all s > 0. The fractional case modifies this by in essence replacing the variable *s* by  $s^{\alpha}$  and indicates that it might to some degree and under certain circumstances shorten the distance the data has to be analytically continued in order to recover the zeros and poles of  $\hat{b}$ . In order to explore this further we will look at a slightly different version of the above uniqueness result that will involve the solution representations of the previous section and provide more insight.

The challenge is to recover both  $\{\lambda_j\}$  and  $\{\rho_j\}$  uniquely from the representations such as 13 and. 15. Once this has been achieved then Corollary 3.1 shows that there is a unique *q* satisfying 1 with 2 for t > T. In addition, as we saw in the previous section, there is a well-proven reconstruction algorithm for recovering q(x) from the spectral data.

One cannot expect the recovery of the  $\{\lambda_j \gamma_j\}$  to be well-posed and the case  $\alpha = 1$  illustrates the difficulties. Now  $E_{1,1}(z) = e^z$  and so in the parabolic case of  $\alpha = 1$  becomes

$$b(t) = \sum_{j=1}^{\infty} \gamma_j \int_0^t e^{-\lambda_j(t-\tau)} a(\tau) d\tau = \sum_{j=1}^{\infty} \beta_j e^{-\lambda_j t} \quad \text{for } t > T.$$

$$(22)$$

where  $\beta_j = \gamma_j \int_0^T e^{\lambda_j \tau} a(\tau) d\tau$ . Equation 22 is a Dirichlet series from which the coefficients  $\{\beta_j, \lambda_j\}$  can be uniquely determined. This can be seen by taking Laplace transforms; the values of  $\lambda_j$  are identified as the locations of the poles of  $\hat{b}$  and  $\beta_j$  as the residues at these poles. From this, in theory,  $\phi'_j(1)$  can be found from  $\beta_j$  which be recovered once  $\lambda_j$  is determined. Solving the Dirichlet series for its component terms is a notoriously ill-posed problem (as it should since it is tantamount to analytic continuation). In addition, while recovering  $\phi_j$  from  $\beta_j$  is mathematically obvious once we have  $\lambda_j$ , the coupling constant is  $\int_0^T e^{\lambda_j \tau} a(\tau) d\tau$  which grows exponentially with *j* (and with *T*) so the computational feasibility is another matter entirely. This will severely restrict both the maximum interval of support [0, T] as well as the number of frequencies  $\lambda_i$  that can be obtained.

On the other hand, when  $\alpha < 1$ , Lemma 2.3 shows that the Mittag-Leffler function has only polynomial growth for large, negative arguments and so we might expect that the fractional diffusion case will be less severely conditioned than the parabolic as in [10], and for this to be more evident the smaller the fractional exponent  $\alpha$ . We shall investigate this in the next section.

## 4 Reconstructing the spectral data

We shall examine a few special cases for the data a(t).

Take a(t) = 1 in (0, T). Reverting back to  $\alpha \le 1$  in the representation 22 and Using 5 with  $\beta = 1 + \alpha$  and  $x = t - \tau$  in gives

$$b(t) = -\sum_{j=1}^{\infty} \gamma_j \int_0^T \frac{d}{d\tau} \left[ (t-\tau)^{\alpha} E_{\alpha,\alpha+1} (-\lambda_j (t-\tau)^{\alpha}) \right] d\tau$$
  
$$= -\sum_{j=1}^{\infty} \gamma_j (t-\tau)^{\alpha} E_{\alpha,\alpha+1} (-\lambda_j (t-\tau)^{\alpha}) \Big|_{\tau=0}^{\tau=T}$$
(23)

Suppose the goal is to recover the first *N* elements of the spectral sequence pair  $\{\gamma_j, \lambda_j\}_{j=1}^N$  from 23. Then we define  $F : \mathbb{R}^{2N} \to C(T, \infty)$  by *F* corresponding to the first *N* terms on the right hand side of 23

$$F(\{\lambda_j, \phi_j'(1)\}_1^N) = \sum_{j=1}^N \gamma_j \left[ t^{\alpha} E_{\alpha, \alpha+1}(-\lambda_j t^{\alpha}) - (t-T)^{\alpha} E_{\alpha, \alpha+1}(-\lambda_j (t-T)^{\alpha}) \right]$$
  
$$=: \sum_{j=1}^N \gamma_j K_{\alpha}(t, \lambda_j)$$
(24)

We then seek a solution of the nonlinear equation

$$F(\{\lambda_{i}, \phi_{i}'(1)\}_{1}^{N}) = b(t)$$
(25)

for the eigenvalues and endpoint values. Note that the range of F is in fact analytic so that in the values over any time interval suffices in theory to determine the values for all complex t. However, we are now interested in the question of a feasible reconstruction of the spectral data and it may seem that choosing a large range of t values will give a more accurate representation of the series especially under a situation where the measured values of b are subject to uncertainty.

The function  $K_{\alpha}(t,\lambda)$  has the same large *t* asymptotic behaviour for all  $\alpha$ ; from 7 we see that  $E_{\alpha,\alpha+1}(-z) = \frac{1}{\Gamma(1)}\frac{1}{z} + O(\frac{1}{z^2})$  for z > 0. Thus a little algebra shows the kernel  $K_{\alpha}$  can be expected to decay as  $O(t^{-2})$  for t >> T and any  $\alpha < 1$ . That is, the asymptotic decay of  $K_{\alpha}$  is, up to a constant multiplier, independent of  $\alpha$  provided  $\alpha < 1$ . This is in sharp contrast to when  $\alpha = 1$  and shows that taking measurements for large times as a means of recovering eigenvalues beyond the first few is pointless in the classical heat equation as the value of the kernel becomes exponentially small. On the other hand, in the fractional diffusion case such large times are not specifically excluded on this count but there is a difficulty for small values of *t*. While the Mittag-Leffler functions decay of polynomial order for large, negative argument, for small time values, due to the fractional power  $t^{\alpha}$  the values of  $K_{\alpha}(t,\lambda)$  for  $\alpha < 1$  are be less than those for  $\alpha = 1$  indicating an advantage to the parabolic case over this range. This is precisely the effect found in the backwards diffusion problem discussed in [8] and the unknown source location problem from time-data in[14].

However, none of this gives insight into the actual inversion of 24 which would require looking at the derivative of *F* with respect to the parameters  $\{\lambda_i, \gamma_i\}$ .

If we now take  $a(t) = \delta_T(t)$  then the previous constructions become

$$b(\tilde{t}+T) = \sum_{j=1}^{\infty} \gamma_j \tilde{t}^{\alpha-1} E_{\alpha,\alpha}(-\lambda_j \tilde{t}^{\alpha}) \qquad \text{for } \tilde{t} > 0.$$
(26)

In this case the kernel  $K_{\alpha}$  now involves the function  $E_{\alpha,\alpha}(-z)$ . This again has quadratic decay for large positive arguments z the reason being that the term in  $\frac{1}{z}$  of the asymptotic expansion is missing since  $1/\gamma(\beta - \alpha) \to 0$  as  $\beta \to \alpha$ . However, when one takes into account that  $z = t^{\alpha}$  and the additional singular term  $t^{\alpha-1}$  the overall asymptotic behaviour is  $\frac{1}{\Gamma(-\alpha)}t^{-1-\alpha} + O(t^{-1-2\alpha})$  and now is no longer independent of  $\alpha$  and the constant in the leading term approaches zero as  $\alpha \to 1$ .

A natural way to solve 25 or the form 22 for more general a(t), is to use Newton's method. Computation of the derivative map is possible from the representation 23. We also have a reasonable starting approximation since we know the asymptotic behaviour of both spectral sequences and the asymptotic values are obtained to a high degree of approximation for even relatively small N provided q is smooth. As we will see, unless we have definite prior information about q, this is an assumption that will be forced on us due to the inevitable ill-conditioning of the problem. In fact, the above suggests that computing the derivative about the approximation q = 0 should give the essential features of the problem and this simplification has been a fairly standard approach for this type of situation, [13, 7, 8].

As we must expect, the greatest difficulty lies in the extraction of the eigenvalues and so we will look at the  $M \times N$  submatrix  $\frac{\partial F}{\partial \lambda}$  where we assume that M *t*-values have been given over a subset of  $(T,\infty)$  and the values of  $\gamma_j$  are held at their asymptotic value. This computation requires evaluating the derivative of  $E_{\alpha,\alpha+1}(-\lambda t^{\alpha})$  with respect to  $\lambda$ . In the case  $a(t) = \delta_T(t)$  we would obtain  $E_{\alpha,\alpha}(-\lambda t^{\alpha})$ . From 6 with  $\beta = 1 + \alpha$  we obtain

$$\frac{\partial}{\partial\lambda}E_{\alpha,\alpha+1}(-\lambda s^{\alpha}) = \frac{s^{\alpha}}{\alpha\lambda} \left[\alpha E_{\alpha,\alpha+1}(-\lambda s^{\alpha}) - E_{\alpha,\alpha}(-\lambda s^{\alpha})\right]$$
(27)

Suppose now we have obtained the sequences  $\{\lambda_j, \gamma_j\}_1^N$  for some *N* where  $\gamma_j = [\phi'_j(1)/||\phi_j||]^2$ . Then it is quite straightforward to reconstruct a potential  $q_N(x)$  from this data. We make the ansatz that  $\{\lambda_j, \gamma_j\}_{j=N+1}^{\infty}$  are given by our best estimate of these values for a fixed potential; The latter can be taken to be for q = 0; a better option is for  $q(x) = \bar{q} := \int_0^1 q(s) ds$  where  $\bar{q}$  can be estimated from  $\bar{q} \approx \lambda_N - N^2 \pi^2$  This estimate will be reasonable for modest size q and relatively small N provided q is smooth, but degenerates outside of these conditions, see [13].

The reconstruction from spectral data can be viewed as only mildly ill-conditioned amounting to effectively only a derivative loss, or in terms of the spectral data, control in the finite dimensional  $H^1$  norm controls q in  $L^2(0, 1)$ , [11, 13]. However from a reconstruction perspective this is not the complete story. The asymptotic behaviour  $\lambda_n = n^2 \pi^2 + \bar{q} + c_n(q)$  where  $c_n = O(n^{-k+2})$  for  $q \in C^k[0,1]$ , shows that the information term  $c_n$  is very small in comparison with the masking term  $n^2\pi^2$ . For even a modestly smooth q, say  $q \in C^2[0,1]$ , this "signal to background" ratio can be easily of order  $10^6 - 10^7$  for n = 10 and only an order of magnitude more for n = 5, see [13]. While a smooth function may not require as many Fourier modes for a reasonable reconstruction, it does show that errors made in computing  $\{\lambda_n\}$  will be magnified considerably when applied to  $\{c_n\}$  and it is this sequence that holds the information on q.

For the above reason, the reconstruction method of first reducing to an inverse spectral problem, then recovering q from spectral data is not optimal. The inversion of 25 to obtain  $\{\lambda_j, \gamma_j\}$  is severely ill-posed and a regularization step must be applied. One can certainly use truncated SVD but this is a rather blunt tool in this context. Tikhonov regularization not only requires estimating the regularization parameter but also requires penalizing in some norm. For the case of the  $\{\lambda_n\}$  recovery we can build in the masking term  $n^2\pi^2$  and a prior assumption about the decay of the coefficients  $\{c_k\}$  based on an assumption about the smoothness of q. This means solving not for the eigenvalues themselves but writing  $\lambda_j = j^2\pi^2 + c_j$  in the definition of F in 25. This is less straightforward than simply penalizing against what prior information one has on q directly. There is another aspect; the representation 25 in any of its forms is valid only for t > T. This is true even for the case  $\alpha = 1$  as 22 shows. This restriction is not essential for the uniqueness proof provided we avoid negative eigenvalues and this can be done by assuming a lower bound for q. The next section will give a more direct reconstruction algorithm and show that there is a considerable advantage to measuring the flux b(t) as early as possible.

## **5** Reconstructing the potential

Let u(x,t;q) be the solution to 1 for a given  $q(x) \in L^2(0,1)$ . Then define the map  $\mathscr{F}(q)$  by

$$\mathscr{F}(q) = -u_x(1,t;q), \quad \text{for } t \in I_t$$
(28)

and we must solve  $\mathscr{F}(q) = b(t)$ . Here  $I_t$  is the measurement interval over which we measure the flux  $u_x(1,t)$ . This can be the interval  $(T,T_f]$  for some fixed final time  $T_f$  as stated originally, or  $(0,T_f)$  as suggested at the end of the last section.

Following the line from the previous section, we propose to solve this by Newton's method. This requires a computation of  $\frac{\partial}{\partial a}\mathscr{F}$  and it is easily seen that  $\frac{\partial}{\partial a}\mathscr{F}[q]$ .  $\delta q$  is the solution of

$$D_t^{\alpha} v(x,t) - v_{xx}(x,t) + q(x)v(x,t) = -\delta q(x)u(x,t;q_n), \qquad 0 < x < 1, \quad t > 0$$
  

$$v(0,t) = 0, \quad v(1,t) = 0, \qquad t > 0$$
  

$$v(x,0) = 0, \quad 0 \le x < \le 1$$
(29)

Then from an initial approximation  $q_0(x)$  we have the following recursion scheme to define  $q_n(x)$ 

$$\frac{\partial}{\partial q}\mathscr{F}[q].\delta q = b(t) - \mathscr{F}[q_n], \qquad q_{n+1} = q_n + \delta q.$$
(30)

We can also look at the special case of a "frozen Newton Scheme" where the derivative is held at a fixed value of q(x), in particular when q = 0. This leads to a formulation very close to that of the previous section. It also allows us to analyze the derivative of  $\mathscr{F}$  as a function of  $\alpha$  which is a primary goal.

To this end we assume that q(x) can be represented by a set of basis functions  $\mathscr{B} = {\{\psi_n(x)\}_1^N}$  for suitably chosen  $\psi_n(x)$ , We thus evaluate  $\mathscr{F}[q=0]$  over a set of M sample points on the interval  $I_t$  for a fixed function a(t) with support on [0,T] and where the directions  $\delta q$  are taken from  $\mathscr{B}$ . Our goal is investigate the distribution of the singular values of the corresponding matrix

$$J_{\alpha} = \mathscr{F}[0]. \psi_k(t_j), \qquad t_j \in I_t, \quad 1 \le k \le N$$

as the fractional derivative constant  $\alpha$  takes on values in (0, 1].

We should make some comment on time scales. In 1 physical constants have been normalized to unity. In particular, it is rescaled with a unit diffusion coefficient and a more physically accurate version would incorporate a diffusion coefficient c(x) in the elliptic operator, that is,  $D_t^{\alpha}u(x,t) - c(x)u_{xx}(x,t) +$ q(x)u(x,t) = 0. This coefficient might itself be a ratio of conductivity and specific heat and can vary considerably from material to material. Typically it will be much smaller than unity (see for example the discussion in [8, Section 3.1]) and this rescaling affects the potential q(x) and the spectrum of the elliptic operator. If these are kept at the normalized values they in turn affect the time scales under consideration – and there will be an  $\alpha$ -dependence here. We shall ignore this and choose to work with a unit coefficient recognizing that from a physical perspective this leads to inflated time scales.

Figure 1 shows the singular values of  $J_{\alpha}$  for  $\alpha = \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1$  when T = 1 and  $I_t = (1, 2]$  where a(t) is taken to be the function  $a(t) = \sin^3(\frac{\pi}{T}t)$ . Sampling within the measurement interval  $I_t$  was taken at every  $\delta t$ ; the leftmost figure shows the case  $\delta t = 0.001$ , the rightmost the case  $\delta t = 0.05$ . Note that we are only seeking 10 modes from the linearized map so that both of these are oversampling, although the leftmost figure exceeds this by a considerable amount. This illustrates the extreme, likely exponential order, ill-conditioning of the problem for all values of  $\alpha$  and this increases with decreasing  $\alpha$ .



Figure 1: Singular values of  $J_{\alpha}$  for  $\alpha = \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1$ .  $T = 1, I_t = (1, 2]$ . Sampling within  $I_t$  was at every  $\delta t$ ; the leftmost figure has  $\delta t = 0.001$ , the rightmost  $\delta t = 0.05$ .

The explanation for this difference is as follows. For the heat equation we are trying to extract the values of  $\lambda_j$  from  $e^{-\lambda_j t_k}$ . If  $t_1$ , the lowest sampled value, is large enough so that  $e^{-\lambda_j t_1} < \delta$  where  $\delta$  is a measure of our measurement accuracy to handle small values then we will be unable to recover this  $\lambda_j$ . The more sample points taken, especially for small value of  $t - T_0$  the better our recovery of, in particular, the larger eigenvalues. Note also that the coefficient  $\gamma_j$  will decrease with  $\lambda_j$  adding to the effect. In the case of  $\alpha < 1$ , for small, negative values of its argument, the Mittag-Leffler function initially decays much faster than the exponential (and this rate increases with decreasing  $\alpha$ ) – again accentuating the phenomenon and providing a rationale for the figures.

If instead of measuring the flux b(t) starting at t = T, that is, immediately after the cut-off value of the support of a(t), we delay for an interval  $T_1, T_2$  where  $T_1 > T$  then the picture changes. The number of recoverable  $\lambda_k$  decreases markedly and especially for the parabolic case  $\alpha = 1$ . This is again what we should expect from the previous discussion. The significant difference is now on the dependence of  $\alpha$ . The rapid decay of the exponential function for even modest values of  $-\lambda t$  severely limits the utility of larger time measurements. In the case of  $\alpha < 1$  the controlling Mittag-Leffler function decays only polynomially for large negative argument and so large time measurements remain useful.

As an example of the above, if we measure only over [1.5T, 3T] (with T = 1) then all singular values  $\sigma_k$  for  $k \ge 3$  are less than  $10^{-10}$ ; the first two singular values are approximately  $10^{-2.2}$  and  $10^{-4.3}$ . For  $\alpha = \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$  the first 3 singular values are greater than  $10^{-7}$  and the decay for the larger index singular values becomes asymptotically nearly independent of  $\alpha$  and significantly greater than that for the case  $\alpha = 1$  as should be expected from the asymptotic behaviour of the Mittag-Leffler function. However, the magnitude of these singular values are still sufficiently small to make the corresponding singular vectors unusable in almost any practical application. For  $\alpha = \frac{3}{4}$  the first four singular values are approximately  $10^{-1.1}, 10^{-3.3}, 10^{-5.8}, 10^{-7.5}$ . Thus if a rough approximation is sufficient this is possibly obtainable in the fractional case, but unlikely in the classical. On the other hand for an immediate measurement, especially with a high sampling rate, the opposite is true,

This reversal of the effective conditioning of the cases  $\alpha < 1$  and  $\alpha = 1$  is similar to the situation with the backwards diffusion problem noted in [8] – although more complex.

In conclusion, one can see that while equations 1 with 2 gives a unique potential q(x) the inverse problem is severely ill-posed. This is yet another example of the "folk theorem:" that a problem where the data is given in one direction (here time) and the unknown (here q(x)) is given in an orthogonal direction is almost certain to be severely ill-conditioned, [3]. Here the reason for this ill-conditioning comes in through each of the reconstruction methods. In the first, analytic continuation was used to obtain spectral information on the operator  $\mathcal{L}u := -u_{xx} + qu$ , thereafter converting the inversion into a mildly ill-conditioned one of known type. In the second, a direct conversion method was used and the linearization of the associated map formed. The inversion of this map is equivalent to a problem that is known to be severely ill-conditioned.

# 6 Acknowledgment

The work of the first author was supported in part by the National Science Foundation through award DMS-1620138. The work of the second author was supported by JSPS KAKENHI Grant Number JP15H05740 and by the A3 Foresight Program Modeling and Computation of Applied Inverse Problems, Japan Society for the Promotion of Science (JSPS).

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