Applied Mathematics and Computation 327 (2018) 70–78

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Numerical inversion of the Laplace transform and its application to fractional diffusion

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ARTICLE INFO

MSC:
44A10
65D32
65M30
33C45

Keywords:
Laplace transform
Quadrature
Inverse Laplace transform
Laguerre polynomials
Fractional diffusion

ABSTRACT

A procedure for computing the inverse Laplace transform of real data is obtained by using a Bessel-type quadrature which is given in terms of Laguerre polynomials $L_N^{(\alpha)}(x)$ and their zeros. This quadrature yields a very simple matrix expression for the Laplace transform $g(s)$ of a function $f(t)$ which can be inverted for real values of s. We show in this paper that the inherent instability of this inversion formula can be controlled by selecting a proper set of the parameters involved in the procedure instead of using standard regularization methods. We demonstrate how this inversion method is particularly well suited to solve problems of the form $\mathcal{L}^{-1}[s\,g(s);t] = f'(t) + f(0)\,\delta(t)$. As an application of this procedure, numerical solutions of a fractional differential equation modeling subdiffusion are obtained and a mean-square displacement law is numerically found.

1. Introduction

The numerical inversion of the Laplace transform on the real axis is an old and difficult problem. A large number of papers have been written on this matter and it stands as a challenge for the community of scientific computing. There are several approaches for solving this ill-posed inverse problem (see for example [1–5] references therein). Since it is a truly ill-conditioned problem, the use of regularization methods is a popular way to reduce the amplification of the errors.

In this paper we present a simple formula for computing the inverse Laplace transform of real data without using regularization methods. This formula is obtained by using a quadrature of a Bessel-type integral transform yielded by the three-term recurrence equation of Laguerre polynomials $L_N^{(\alpha)}(x)$, as well as their asymptotic expressions and a bilinear generating function; it converges as $\mathcal{O}(1/N)$ for continuous functions under certain integral conditions [6,7] and yields a quadrature for the Laplace transform

$$g(s) = \mathcal{L}[f(x); s] = \int_0^\infty e^{-sx} f(x) dx. \tag{1}$$

Evaluating this quadrature at M points $0 < s_1 < s_2 < \cdots < s_M$ we obtain a linear system that can be inverted to give a formula for the inverse Laplace transform. Instead of using a regularization method for solving this ill-conditioned system, we control the instability by taking advantage of the lack of specific values of the nodes s_k, $k = 1, 2, \ldots, M$ and the number N of the quadrature nodes. It is shown below that this inversion formula can be used to obtain the inverse Laplace transform in

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https://doi.org/10.1016/j.amc.2018.01.026

problems of the form $\mathcal{L}^{-1}[s\,g(s);t] = f'(t) + f(0)\,\delta(t)$. Finally, as an application, we also show that this formula can be used to solve a fractional differential equation modelling the subdiffusion process and to compute the mean-square displacement $\langle x^2(t)\rangle$.

2. Discrete Laguerre functions

Let us begin with a review of some important facts about the discrete Laguerre functions [6,8]. The recurrence equation satisfied by the Laguerre polynomials is

$$-(n+1)L_{n+1}^{\alpha}(x) + (2n+\alpha+1)L_n^{\alpha}(x) - (n+\alpha)L_{n-1}^{\alpha}(x) = xL_n^{\alpha}(x), \tag{2}$$

where $\alpha > -1$ and $n = 0, 1, \ldots$. This equation can be written as the following spectral problem:

$$\begin{pmatrix} \alpha+1 & -1 & 0 & \cdots \\ -(\alpha+1) & \alpha+3 & -2 & \cdots \\ 0 & -(\alpha+2) & \alpha+5 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} L_0^{\alpha}(x) \\ L_1^{\alpha}(x) \\ L_2^{\alpha}(x) \\ \vdots \end{pmatrix} = x \begin{pmatrix} L_0^{\alpha}(x) \\ L_1^{\alpha}(x) \\ L_2^{\alpha}(x) \\ \vdots \end{pmatrix}. \tag{3}$$

The eigenproblem associated to the principal submatrix of dimension N of (3)

$$\begin{pmatrix} \alpha+1 & -1 & \cdots & 0 \\ -(\alpha+1) & \alpha+3 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 2N+\alpha-1 \end{pmatrix} \begin{pmatrix} u_{0k} \\ u_{1k} \\ \vdots \\ u_{N-1,k} \end{pmatrix} = x_k \begin{pmatrix} u_{0k} \\ u_{1k} \\ \vdots \\ u_{N-1,k} \end{pmatrix}, \tag{4}$$

can be solved by a similarity transformation and the Christoffel–Darboux formula for Laguerre polynomials. Thus, we obtain that the eigenvalue x_k is one of the N zeros of $L_N^{\alpha}(x)$ and the nth entry of kth eigenvector is given by

$$u_{nk} = (-1)^{k+1}\left(\frac{n!\,\Gamma(\alpha+N)x_k}{N!\,(N+\alpha)\Gamma(\alpha+n+1)}\right)^{1/2} \frac{L_n^{(\alpha)}(x_k)}{L_{N-1}^{(\alpha)}(x_k)}, \tag{5}$$

$n = 0, 1\ldots, N-1,\ k = 1, 2, \ldots, N$. By using the asymptotic formula [9]

$$L_N^{(\alpha)}(x) = \frac{N^{\alpha/2-1/4}e^{x/2}}{\sqrt{\pi}\,x^{\alpha/2+1/4}}\left(\cos(2\sqrt{Nx} - \alpha\pi/2 - \pi/4) + (Nx)^{-1/2}\mathcal{O}(1)\right) \tag{6}$$

and the fact that x_k is a zero of $L_N^{\alpha}(x)$, one can see that (5) approaches the Laguerre function

$$\varphi_n^{\alpha}(x) = c_n\, e^{-x/2}x^{\alpha/2+3/4}L_n^{\alpha}(x)$$

evaluated at x_k, for sufficiently large values of N and fixed k. Here, c_n is a constant depending on N and α.

3. A Bessel transform

Let U be the orthogonal matrix whose entries are u_{nk}, as given by (5). Let us define the matrix

$$T(z) = U^t D(z) U,$$

where $D(z)$ is the diagonal matrix $D(z) = \mathrm{diag}\{1, z, z^2, \ldots, z^{N-1}\}$ and z is an complex number. Thus, the components of $T(z)$ are given by

$$T_{jk}(z) = \lambda_{jk} \sum_{n=0}^{N-1} \frac{n!\,z^n}{\Gamma(\alpha+n+1)} L_n^{(\alpha)}(x_j)L_n^{(\alpha)}(x_k), \tag{7}$$

where

$$\lambda_{jk} = \frac{(-1)^{j+k}\Gamma(\alpha+N)\sqrt{x_j x_k}}{N!\,(N+\alpha)L_{N-1}^{(\alpha)}(x_j)L_{N-1}^{(\alpha)}(x_k)}. \tag{8}$$

The use of Eq. (6) yields asymptotic expressions for both λ_{jk} and the zeros of $L_N^{(\alpha)}(x)$. Thus, defining the function $\sigma(x) = \sqrt{x}$ we obtain

$$\lambda_{jk} \simeq 2\left(x_j x_k\right)^{\alpha/2+1/4} \exp\left(-\frac{x_j + x_k}{2}\right)\Delta\sigma(x_k)$$

and

$$x_k \simeq \frac{\pi^2}{4N}(k + \alpha/2 - 1/4)^2, \quad k = 1, 2\ldots, N. \tag{9}$$