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On numerical contour integral method for fractional diffusion equations with variable coefficients

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ABSTRACT

In this note, we study numerical contour integral method for fractional diffusion equations with variable coefficients. We find that the method can be applied if the diffusion coefficients and order of differentiation satisfy a certain condition. This work extends a recent result.

1. Introduction

Consider the following space-fractional diffusion equation:

$$\frac{\partial u(x,t)}{\partial t} = d_1(x)\frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha} + d_2(x)\frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha} + b(x,t), \quad x \in (x_L, x_R),\ t \in (0,T], \tag{1.1}$$

$$u(x_L,t) = u(x_R,t) = 0, \quad t \in (0,T], \qquad u(x,0) = u_0(x), \quad x \in [x_L, x_R], \tag{1.2}$$

where $1 < \alpha < 2$ and the diffusion coefficients $d_1(x)$, $d_2(x)$ are nonnegative functions.

The left-sided and right-sided fractional derivatives $\frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha}$ and $\frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha}$ can be defined in the Grünwald–Letnikov form [1]:

$$\frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha} = \lim_{\Delta x \to 0^+} \frac{1}{\Delta x^\alpha} \sum_{k=0}^{\lfloor (x-x_L)/\Delta x \rfloor} g_k^{(\alpha)} u(x - k\Delta x, t),$$
$$\frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha} = \lim_{\Delta x \to 0^+} \frac{1}{\Delta x^\alpha} \sum_{k=0}^{\lfloor (x_R-x)/\Delta x \rfloor} g_k^{(\alpha)} u(x + k\Delta x, t),$$

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where $\lfloor y \rfloor$ represents the floor of y, and $g_k^{(\alpha)} = (-1)^k \binom{\alpha}{k}$ with $\binom{\alpha}{k}$ being the fractional binomial coefficients. Since fractional derivatives are nonlocally defined, lots of works have been done on fast method for solving the problem by time-stepping method, see [2–4] and the reference therein.

In this note, we consider solving (1.1), (1.2) numerically by contour integral method. The method has been shown to be an efficient alternative of the time stepping method for solving different kinds of problems [5–7]. Notice that, when (1.1), (1.2) are discretized, one needs to solve ordinary differential equation (ODE) of the following form:

$$d\mathbf{u}(t)/dt = A\mathbf{u}(t) + \mathbf{b}(t), \quad \mathbf{u}(0) = \mathbf{u}_0, \tag{1.3}$$

where $A \in \mathbb{R}^{n\times n}$, $\mathbf{u}(t)$, $\mathbf{u}_0$ and $\mathbf{b}(t) \in \mathbb{R}^n$. Numerical contour integral method (see [8,9]) with hyperbolic contour $z(\zeta) = \mu[1+\sin(\mathbf{i}\zeta-\theta)]$ $(\zeta \in (-\infty,\infty))$ can be used to solve (1.3), where $\mu > 0$ and θ are parameters to be determined. The solution is approximated by $\mathbf{u}(t) \approx \frac{h}{\pi}\mathrm{Im}\left\{\sum_{k=0}^{N-1} e^{z_k t} z_k' \hat{\mathbf{u}}_k\right\}$, with $\mathbf{i} = \sqrt{-1}$, $z_k = z(\zeta_k)$, $z_k' = z'(\zeta_k)$ and $\zeta_k = (k+\frac{1}{2})h$. Here h is the uniform space node, N is the number of quadrature nodes, and the vectors $\hat{\mathbf{u}}_k$ $(k = 0,1,\ldots,N-1)$ are solutions to the linear systems $(z_k I - A)\hat{\mathbf{u}}_k = \mathbf{u}_0 + \hat{\mathbf{b}}(z_k)$, in which I is the identity matrix and $\hat{\mathbf{b}}(\cdot)$ is the Laplace transform of $\mathbf{b}(\cdot)$.

The hyperbolic contour integral can be applied if all the singularities fall into a sectorial region $\Sigma_\delta = \left\{z \in \mathbb{C} : |\arg(-z)| \le \delta, \delta \in \left(0, \frac{\pi}{2}\right), \text{ and } z \neq 0\right\}$. In this situation, optimal values of h, μ and θ can be determined by the value of δ. Moreover, discretization error is bounded by

$$\frac{1}{2\pi(e^{2\pi\nu_+/h}-1)} \max_{-\infty<\zeta<+\infty}\left\{\|(z(\omega)I-A)^{-1}\|\|\tilde{\mathbf{b}}(z(\omega))\|\right\}\int_{-\infty}^{\infty}|e^{z(\omega)t}z'(\omega)|d\zeta, \tag{1.4}$$

where $\nu_+ > 0$, $\omega = \zeta + \mathbf{i}\nu_+$, $\tilde{\mathbf{b}}(z(\omega)) = \mathbf{u}_0 + \hat{\mathbf{b}}(z(\omega))$ and $\|\cdot\|$ is some matrix norm. We refer interested readers to [8,9] for details. One may also refer to [10,11] for sectorial property of fractional operator.

In [8], it was shown the method works well numerically but was theoretically supported only under the condition that $d_2(x) = cd_1(x)$ for some constant c. In the next section, by further studying the relation between generating function of a Toeplitz matrix and its bilinear form, we find, when the diffusion coefficients $d_1(x)$, $d_2(x)$ and the fractional order of the derivative α satisfy a certain condition, a sectorial region in which all singularities locate. As a result, the contour integral method can be applied in this situation.

2. Space-fractional diffusion equations with variable coefficients

To discretize (1.1), (1.2), let $\Delta x = \frac{x_R - x_L}{J+1}$ with J being some given positive integer. For $j = 0,1,\ldots,J+1$, denote $x_j = x_L + j\Delta x$, $u_j(t) = u(x_j,t)$, $d_{l,j} = d_l(x_j)$, $l = 1,2$, and $b_j(t) = b(x_j,t)$. Then using the shifted Grünwald approximations [12], one can obtain the following first order scheme

$$\frac{\partial u_j(t)}{\partial t} = \frac{d_{1,j}}{\Delta x^\alpha}\sum_{k=0}^{j+1} g_k^{(\alpha)} u_{j-k+1}(t) + \frac{d_{2,j}}{\Delta x^\alpha}\sum_{k=0}^{J-j+2} g_k^{(\alpha)} u_{j+k+1}(t) + b_j(t), \quad j = 1,2,\ldots,J.$$

The scheme can be put into ODE matrix form (1.3), where $\mathbf{u}(t) = [u_1(t), u_2(t), \ldots, u_J(t)]^T$, $\mathbf{b}(t) = [b_1(t), b_2(t), \ldots, b_J(t)]^T$ and $A = \frac{1}{\Delta x^\alpha}(D_1 G_\alpha + D_2 G_\alpha^T)$ with $D_1 = \mathrm{diag}(d_{1,1}, d_{1,2}, \ldots, d_{1,J})$, $D_2 = \mathrm{diag}(d_{2,1}, d_{2,2}, \ldots, d_{2,J})$ and

$$G_\alpha = \begin{bmatrix} g_1^{(\alpha)} & g_0^{(\alpha)} & 0 & \cdots & 0 & 0 \\ g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} & 0 & \cdots & 0 \\ \vdots & g_2^{(\alpha)} & g_1^{(\alpha)} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ g_{J-1}^{(\alpha)} & \ddots & \ddots & \ddots & g_1^{(\alpha)} & g_0^{(\alpha)} \\ g_J^{(\alpha)} & g_{J-1}^{(\alpha)} & \cdots & \cdots & g_2^{(\alpha)} & g_1^{(\alpha)} \end{bmatrix}. \tag{2.1}$$