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Spectral analysis and structure preserving preconditioners for fractional diffusion equations

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A B S T R A C T

Fractional partial order diffusion equations are a generalization of classical partial differential equations, used to model anomalous diffusion phenomena. When using the implicit Euler formula and the shifted Grünwald formula, it has been shown that the related discretizations lead to a linear system whose coefficient matrix has a Toeplitz-like structure. In this paper we focus our attention on the case of variable diffusion coefficients. Under appropriate conditions, we show that the sequence of the coefficient matrices belongs to the Generalized Locally Toeplitz class and we compute the symbol describing its asymptotic eigenvalue/singular value distribution, as the matrix size diverges. We employ the spectral information for analyzing known methods of preconditioned Krylov and multigrid type, with both positive and negative results and with a look forward to the multidimensional setting. We also propose two new tridiagonal structure preserving preconditioners to solve the resulting linear system, with Krylov methods such as CGNR and GMRES. A number of numerical examples show that our proposal is more effective than recently used circulant preconditioners.

1. Introduction

Fractional-space diffusion equations (FDEs) are used to describe diffusion phenomena, that cannot be modeled by the second order diffusion equations. More precisely, when a fractional derivative replaces a second derivative in a diffusion model, it leads to enhanced diffusion. The FDEs are of numerical interest, since there exist only few cases in which the analytic solution is known. As a consequence, in the past ten years, many methods have been proposed for solving numerically FDEs problems. In [16,17] Meerschaert and Tadjeran introduced an unconditionally stable method for approximating the FDEs: from a numerical linear algebra viewpoint, it is worth noticing that the resulting linear systems show a strong structure and indeed the related coefficient matrices can be seen as a sum of two diagonal times Toeplitz matrices (see [32]). Exploiting such a structure, in [31] the authors employed the conjugate gradient normal residual (CGNR) method and numerically showed that its convergence is fast when the diffusion coefficients are small, that is in this case the resulting linear system is well-conditioned. On the other hand, when the diffusion coefficients are not small, the problem becomes ill-conditioned and the convergence of the CGNR method slows down. To avoid the resulting drawback, in [19] Pang and Sun proposed a multigrid method that converges very fast, even in the ill-conditioned case. The linear convergence of such

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a method has been proved only in the case of constant and equal diffusion coefficients. With the same purpose, Lei and Sun used the CGNR method with a circulant preconditioner and verified that it converges superlinearly (see [15]), again in the case of constant diffusion coefficients. A further improvement of the circulant preconditioning has been proposed in [18]. Both strategies preserve the computational cost per iteration of $O(N \log N)$ operations, typical of the CGNR method when applied to Toeplitz type structures.

Under appropriate conditions, in this paper we show that the coefficient matrix-sequence coming from the Meerschaert–Tadjeran method belongs to the Generalized Locally Toeplitz (GLT) class [25,26] and we compute the associated symbol: it turns out that the symbol describes the asymptotic singular value distribution, as the matrix size tends to infinity. In other words, an evaluation of the symbol over a uniform equispaced gridding in the domain leads to a reasonable approximation of the singular values, when the matrix size is sufficiently large. Furthermore, when the diffusion coefficients are equal (even if not necessarily constant), we show that the symbol also describes the eigenvalue distribution. Making use of such asymptotic spectral information, we study in more detail recently developed techniques, by furnishing new positive and negative results: for instance we prove that the circulant preconditioning described in [15] cannot be superlinear in the variable coefficient case, due to a lack of clustering at a single point, while the multigrid approach based on the symbol (which goes back to [9,2] and it is used in this FDE context in [19]) can be optimal also in the variable coefficient setting. We finally introduce two tridiagonal preconditioners for Krylov methods like CGNR and GMRES, which preserve the Toeplitz-like structure of the coefficient matrix. One of the preconditioners involves the first derivative discretization matrix and is suitable for fractional exponents close to 1, the other makes use of the discrete Laplacian matrix and is recommended for fractional exponents close to 2. Due to their tridiagonal structure, both preconditioners preserve the computational cost per iteration of the used Krylov method. A clustering analysis of the preconditioned matrix-sequences, even in case of nonconstant diffusion coefficients, is also provided.

The paper is organized as follows. In Section 2 we briefly introduce the FDEs equations and recall the Meerschaert–Tadjeran discretization. Section 3 concerns the symbol and the spectral distribution of the resulting coefficient matrix-sequence. In Section 4 we study known preconditioning techniques and multigrid methods by using the spectral information and we give details on our new preconditioning strategy. Finally, Section 5 is devoted to numerical examples and Section 6 contains conclusions and open problems.

2. Fractional diffusion equations and a finite difference approximation

We are interested in the following initial-boundary value problem

$$\begin{cases} \frac{\partial u(x,t)}{\partial t} = d_+(x,t)\frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha} + d_-(x,t)\frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha} + f(x,t), & (x,t) \in (L,R)\times(0,T], \\ u(L,t) = u(R,t) = 0, & t \in [0,T], \\ u(x,0) = u_0(x), & x \in [L,R], \end{cases} \tag{1}$$

where $\alpha \in (1,2)$ is the fractional derivative order, $f(x,t)$ is the source term and the nonnegative functions $d_\pm(x,t)$ are the diffusion coefficients. The right-handed ($-$) and the left-handed ($+$) fractional derivatives in (1) are defined in Riemann–Liouville form as follows

$$\frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha} = \frac{1}{\Gamma(n-\alpha)}\frac{\partial^n}{\partial x^n}\int_L^x \frac{u(\xi,t)}{(x-\xi)^{\alpha+1-n}}d\xi,$$

$$\frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha} = \frac{(-1)^n}{\Gamma(n-\alpha)}\frac{\partial^n}{\partial x^n}\int_x^R \frac{u(\xi,t)}{(\xi-x)^{\alpha+1-n}}d\xi,$$

where n is an integer such that $n-1 < \alpha \le n$ and $\Gamma(\cdot)$ is the gamma function. If $\alpha = m$, with $m \in \mathbb{N}$, the fractional derivatives reduce to the standard integer derivatives, i.e.,

$$\frac{\partial^m u(x,t)}{\partial_+ x^m} = \frac{\partial^m u(x,t)}{\partial x^m}, \quad \frac{\partial^m u(x,t)}{\partial_- x^m} = (-1)^m\frac{\partial^m u(x,t)}{\partial x^m}.$$

Let us observe that when $\alpha = 2$ the equation in (1) reduces to a parabolic partial differential equation (PDE), while when $\alpha = 1$ it becomes a hyperbolic PDE. From a numerical point of view, an interesting definition of the fractional derivatives is the shifted Grünwald definition given by

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

$$\frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha} = \lim_{\Delta x\to 0^+}\frac{1}{\Delta x^\alpha}\sum_{k=0}^{\lfloor (R-x)/\Delta x\rfloor} g_k^{(\alpha)} u(x+(k-1)\Delta x,t), \tag{2}$$