Spectral analysis and numerical methods for fractional diffusion equations

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Fractional Diffusion Equations (FDEs)

We are interested in the following space-fractional diffusion equation (FDE)

$$\frac{\partial u(x,t)}{\partial t} = d_+(x,t)\frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha} + d_-(x,t)\frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha} + f(x,t),$$

where

- $\alpha \in (1,2)$ is the fractional derivative order,
- $d_\pm(x,t) \geqslant 0$ are the diffusion coefficients,
- $(x,t) \in (L,R) \times (0,T]$, with the initial-boundary conditions

$$\begin{cases} u(L,t) = u(R,t) = 0, & t \in [0,T], \\ u(x,0) = u_0(x), & x \in [L,R]. \end{cases}$$

Anomalous diffusion

- $\alpha = 2 \Rightarrow$ parabolic PDE
- Fractional space derivatives are used to model anomalous diffusion or dispersion, where a particle plume spreads at a rate inconsistent with the classical Brownian motion model.
- Replacing the second derivative in a diffusion or dispersion model with a fractional derivative it leads to enhanced diffusion (super-diffusion).
- Applications: hydrology, finance, image processing, ...

Fractional Diffusion Equations (FDEs)

$\frac{\partial^\alpha u(x,t)}{\partial_\pm x^\alpha}$ are defined by the shifted Grünwald formula

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

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

where $g_k^{(\alpha)}$ are the alternating fractional binomial coefficients

$$g_k^{(\alpha)} = (-1)^k \left(\begin{array}{c} \alpha \\ k \end{array} \right) = \frac{(-1)^k}{k!}\alpha(\alpha-1)\cdots(\alpha-k+1) \quad k = 0, 1, \ldots$$

A discretization

Fix two positive integers N, M, and define the following partition of $[L, R] \times [0, T]$,

$$\begin{gathered} x_i = L + i\Delta x, \quad \Delta x = \frac{(R-L)}{N+1}, \quad i = 0, \dots, N+1, \\ t_m = m\Delta t, \quad \Delta t = \frac{T}{M}, \quad m = 0, \dots, M, \end{gathered}$$

1. discretization in time by an implicit Euler method
2. discretization in space of the fractional derivatives by the shifted Grünwald formula

$$\Downarrow$$

consistent and unconditionally stable method[1,2].

[1] Meerschaert, Tadjeran, *J. Comput. Appl. Math.*, 2004

[2] Meerschaert, Tadjeran, *Appl. Numer. Math.*, 2006

Matrix form of the discretized problem

$$\left(\nu_{M,N} I + D_+^{(m)} T_{\alpha,N} + D_-^{(m)} T_{\alpha,N}^T\right) u^{(m)} = \nu_{M,N} u^{(m-1)} + \Delta x^\alpha f^{(m)},$$

- $T_{\alpha,N}$ lower Hessenberg Toeplitz matrix

$$T_{\alpha,N} = - \begin{bmatrix} g_1^{(\alpha)} & g_0^{(\alpha)} & 0 & \cdots & 0 & 0 \\ g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ g_{N-1}^{(\alpha)} & \ddots & \ddots & \ddots & g_1^{(\alpha)} & g_0^{(\alpha)} \\ g_N^{(\alpha)} & g_{N-1}^{(\alpha)} & \cdots & \cdots & g_2^{(\alpha)} & g_1^{(\alpha)} \end{bmatrix}_{N \times N}$$

- $D_\pm^{(m)} = \mathrm{diag}(d_{\pm,1}^{(m)}, \ldots, d_{\pm,N}^{(m)})$ with $d_{\pm,i}^{(m)} := d_\pm(x_i, t_m)$
- $\nu_{M,N} = \frac{\Delta x^\alpha}{\Delta t}$
- $f^{(m)}, u^{(m)} \in \mathbb{R}^N$, with $f_i^{(m)} := f(x_i, t_m)$, and $u_i^{(m)} \approx u(x_i, t_m)$

Preliminaries: symbol

Def1 Let $f \in L^1[-\pi, \pi]$ with Fourier coefficients

$$f_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\theta) e^{-\mathrm{i} j\theta} d\theta, \quad j \in \mathbb{Z}.$$

Then the Toeplitz matrix of size $n \times n$ generated by f is

$$T_n(f) = [f_{i-j}]_{i,j=1}^{n}$$

- The symbol f describes the spectrum of $T_n(f)$ for n large enough:

$$\{T_n(f)\}_{n \in \mathbb{N}} \sim_\lambda (f, [-\pi, \pi])$$

Symbol and spectral distribution of $\left\{\mathcal{M}_{\alpha,N}^{(m)}\right\}_{N\in\mathbb{N}}$

The coefficient matrix

$$\mathcal{M}_{\alpha,N}^{(m)} = \nu_{M,N} I + D_+^{(m)} T_{\alpha,N} + D_-^{(m)} T_{\alpha,N}^T$$

is a symmetric Toeplitz matrix in the case of constant and equal diffusion coefficients ($D_\pm^{(m)} = d \cdot I$, $d > 0$)

If $\nu_{M,N} = o(1)$ then

$$\left\{\mathcal{M}_{\alpha,N}^{(m)}\right\} \sim_\lambda (d \cdot p_\alpha(\theta), [-\pi, \pi]),$$

where

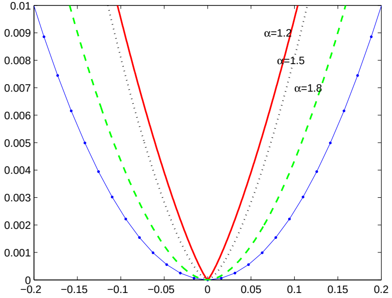
$$p_\alpha(\theta) = f_\alpha(\theta) + f_\alpha(-\theta) = f_\alpha(\theta) + \overline{f_\alpha(\theta)}$$

$$f_\alpha(\theta) = -\sum_{k=-1}^{\infty} g_{k+1}^{(\alpha)} \mathrm{e}^{\mathbf{i}k\theta} = -\mathrm{e}^{-\mathbf{i}\theta}\left(1 - \mathrm{e}^{\mathbf{i}\theta}\right)^{\alpha}.$$

is a real-valued continuous function.

Zero of the symbols $p_\alpha(\theta)$

The function $p_\alpha(\theta)$ has a zero of order $\alpha \in (1,2)$ at 0



Comparison between the symbol of the Laplacian operator $\ell(\theta) = 2 - 2\cos(\theta)$ (**blue** bullet line) with $p_\alpha(\theta)$ for $\alpha = \mathbf{1.2}$ (**red** solid line), $\alpha = \mathbf{1.5}$ (**black** dotted line) and $\alpha = \mathbf{1.8}$ (**green** dashed line) in a neighborhood of 0.

Curiosity $p_1(\theta) = \ell(\theta) = \frac{1}{2} p_2(\theta)$.

Variable coefficients case

Generalized Localy Toeplitz (GLT) matrices[3] combine diagonal and Toeplitz matrices (first proposal in [4])

$$\boxed{\mathcal{M}_{\alpha,N}^{(m)} = \nu_{M,N} I + D_{+}^{(m)} T_{\alpha,N} + D_{-}^{(m)} T_{\alpha,N}^{T}}$$

If $\nu_{M,N} = o(1)$ and $d_{\pm}(x) := d_{\pm}(x, t_m)$ Riemann integrable for a fixed t_m, then

$$\left\{\mathcal{M}_{\alpha,N}^{(m)}\right\} \sim_{\sigma} (h_{\alpha}(x,\theta), [L,R] \times [-\pi,\pi]).$$

$$h_{\alpha}(x,\theta) = d_{+}(x) f_{\alpha}(\theta) + d_{-}(x) f_{\alpha}(-\theta), \quad (x,\theta) \in [L,R] \times [-\pi,\pi],$$

If $d_{+}(x) = d_{-}(x)$, we also have $\left\{\mathcal{M}_{\alpha,N}^{(m)}\right\} \sim_{\lambda} (h_{\alpha}(x,\theta), [L,R] \times [-\pi,\pi])$.

[3] Serra-Capizzano, *LAA*, 2006

[4] Tilli, *LAA*, 1998

2D FDEs

$$\begin{cases} \frac{\partial u(x,y,t)}{\partial t} = d_+(x,y,t)\frac{\partial^\alpha u(x,y,t)}{\partial_+ x^\alpha} + d_-(x,y,t)\frac{\partial^\alpha u(x,y,t)}{\partial_- x^\alpha} & (x,y,t) \in \Omega \times (0,T], \\ \quad + e_+(x,y,t)\frac{\partial^\beta u(x,y,t)}{\partial_+ y^\beta} + e_-(x,y,t)\frac{\partial^\beta u(x,y,t)}{\partial_- y^\beta} + f(x,y,t), & \\ u(x,y,t) = 0, & (x,y,t) \in \partial\Omega \times [0,T], \\ u(x,y,0) = u_0(x,y), & (x,y) \in \bar{\Omega}, \end{cases}$$

Using the second-order accurate CN-WSGD* scheme[5] the coefficient matrix is

$$\mathcal{M}^{(m)}_{(\alpha,\beta),N} = \left(\frac{1}{r} I_N + A_x^{(m)} + \frac{s}{r} A_y^{(m)}\right), \qquad r = \frac{\Delta t}{2\Delta x^\alpha}, \; s = \frac{\Delta t}{2\Delta y^\beta}, \; N = N_1 N_2$$

$$\begin{cases} A_x^{(m)} = D_+^{(m)}(I_{N_2} \otimes T_{\alpha,N_1}) + D_-^{(m)}(I_{N_2} \otimes T^T_{\alpha,N_1}), \\ A_y^{(m)} = E_+^{(m)}(T_{\beta,N_2} \otimes I_{N_1}) + E_-^{(m)}(T^T_{\beta,N_2} \otimes I_{N_1}). \end{cases}$$

We can compute the symbol of $\mathcal{M}^{(m)}_{(\alpha,\beta),N}$ ...

∗ Crank-Nicolson in time and a second order approximation of the Riemann-Liouville fractional derivatives called Weighted and Shifted Grünwald Difference

[5] W. Tian, H. Zhou, W. Deng, *Math. Comp.*, 2015

Preconditioners

- Matrix-vector product with $\mathcal{M}^{(m)}_{(\alpha,\beta),N}$ in $O(N\log(N))$.
- Circulant preconditioner **CANNOT** give a proper clustering in the multidimensional problems also in the constant coefficient setting due to the negative results in [6].
- The preconditioner $P^{(m)}_{2,N} = \mathcal{M}^{(m)}_{(2,2),N}$, i.e., shifted Laplacian,
  - The condition number of the preconditioned matrix $P^{(m)}_{2,N}\mathcal{M}^{(m)}_{\alpha,N}$ is asymptotical to $N^{2-\gamma}$, with $\gamma = \max\{\alpha,\beta\}$ s.t. $0 < 2-\gamma < 1$ [7] $\Rightarrow$ the number of iterations of a conjugate gradient type method grows as $O(N^{\frac{2-\gamma}{2}})$ [8]
    $\Rightarrow$ $P^{(m)}_{2,N}$ is a good choice when α or β are close to 2.
  - only five nonzero diagonals, but the Gaussian elimination is computationally too expensive $\Rightarrow$ Multigrid methods

[6] Serra-Capizzano, Tyrtyshnikov, *SIMAX*, 1999
[7] Serra S., *Calcolo*, 1995

[8] Axelsson O., Lindskog G., *Numer. Math.*, 1986

Algebraic interpretation of Multigrid methods

Multigrid Idea

Project the system in a subspace, solve the resulting system in this subspace and interpolate the solution in order to improve the previous approximation.

Multigrid components

The Multigrid combines two iterative methods:

Smoother: a classic iterative method,

Coarse Grid Correction: projection of the error equation, solution of the restricted problem, interpolation.

Even if the two components have not a good convergence, their combination could results in a very fast iterative method if they are spectrally complementary.

Multigrid methods

Multigrid for 1D constant coefficients FDE was proposed in[9]

- Jacobi smoother and linear interpolation projector.
- The two grid convergence analysis agrees with results for Toeplitz matrices in[10,11].
- The numerical results show a linear convergence rate also for
  - V-cycle,
  - variable coefficients,
  - the coarser matrices are obtained by rediscretization instead of the Galerkin approach.

[9] Pang, Sun, *J. Comput. Phys.*, 2012
[10] Fiorentino, Serra-Capizzano *Calcolo*, 1991

[11] Chan et al., *SISC*, 1998

Our symbol analysis for Multigrid methods

Using the symbol of $\mathcal{M}^{(m)}_{(\alpha,\beta),N}$

- Two-grid convergence analysis for the 2D problem[12] proving: smoothing condition for Jacobi and approximation condition for linear interpolation.
- Constant case: The V-cycle optimality requires[11]

$$\lim_{\theta\to 0} \frac{p(\hat{\theta})}{f(\theta)} = c < \infty, \qquad \hat{\theta} \in V(\theta), \tag{2}$$

  where $V(\theta) = \{(\theta, \theta+\pi), (\theta+\pi, \theta), (\theta+\pi, \theta+\pi)\}$, p is the symbol of the linear interpolation, and f is the symbol of the FDE. Under the assumption $\frac{\Delta x^{\alpha}}{\Delta t} = o(1)$, and constant diffusion coefficients, the (2) holds with $c = 0 \Rightarrow$ the projector is robust (geometric multigrid).
- Nonconstant case: When the diffusion coefficients are uniformly bounded and positive the optimality of the TGM can be proved using[14].

[12] Dehghan et al., manuscript
[13] Aricò, Donatelli, *Numer. Math.*, 2007

[14] Serra-Capizzano, Tablino-Possio, *Calcolo*, 2014

Galerkin and geometric Multigrid methods

- Galerkin approach:
$$A_{k+1} = P_k A_k P_k^T,$$
where A_k and P_k are the coefficient matrix and the projection matrix at the recursion level k.
    - Pro: It is robust and the theory is well-defined
    - Converse: Setup phase for computing all A_k, which could be computational expensive
- Geometric approach: A_k rediscretization of the same FDE at each recursion level.
    - Pro: Cheap and easy to compute
    - Converse: Be careful to scaling and less robust than Galerkin, but $c = 0$ helps!

Numerical results

- We choose $\Delta x = \Delta y = \Delta t$, such that

$$\frac{1}{r} = \frac{2\Delta x^{\alpha}}{\Delta t} = 2\Delta x^{\alpha-1} \xrightarrow{N\to\infty} 0$$

- Compute the average number of iterations as $\frac{1}{M}\sum_{m=1}^{M}\mathrm{Iter}(m)$, where $\mathrm{Iter}(m)$ is the number of iterations at time t_m
- GMRES with tollerance 10^{-7}

Example from[15]: $\alpha = 1.8$, $\beta = 1.9$

$$d_+(x,y,t) = 4(1+t)x^{\alpha}(1+y), \qquad d_-(x,y,t) = 4(1+t)(1-x)^{\alpha}(1+y),$$
$$e_+(x,y,t) = 4(1+t)(1+x)y^{\beta}, \qquad e_-(x,y,t) = 4(1+t)(1+x)(1-y)^{\beta}.$$

on the spatial domain $\Omega = [0,1]\times[0,1]$ and time interval $[0,T] = [0,1]$.

Preconditioners

- P_{ILU} the proposal in [15] based on ILU for the inverse of a band preconditioner (7 bandwidth at blocks with blocks with bandwidth 7)
- P_2 one iteration of Galerkin multigrid applied to $\mathcal{M}^{(m)}_{(2,2),N} \Rightarrow O(N)$
- P_{MGM} one iteration of geometric multigrid applied to the coefficient matrix $\mathcal{M}^{(m)}_{(\alpha,\beta),N}$
- The multigrid methods use one step of Jacobi as pre- and post-smoother, while the grid transfer operator is the bilinear interpolation.

[15] Jin, Lin, Zhao, *Commun. Comput. Phys.* 2015.

Number of iterations

N_1	$GMRES(20)$	P_{ILU}	P_2	P_{MGM}
2^4	48.750	11.000	18.063	9.000
2^5	81.594	12.406	15.813	9.000
2^6	157.750	14.250	11.531	10.000
2^7	273.914	17.055	12.000	9.891

Example 2

- $\alpha = 1.8$, $\beta = 1.6$
- Diffusion coefficients

$$
\begin{aligned}
d_+(x,y,t) &= \Gamma(3-\alpha)(1+x)^{\alpha}(1+y)^{2} \\
d_-(x,y,t) &= \Gamma(3-\alpha)(3-x)^{\alpha}(3-y)^{2} \\
e_+(x,y,t) &= \Gamma(3-\beta)(1+x)^{2}(1+y)^{\beta} \\
e_-(x,y,t) &= \Gamma(3-\beta)(3-x)^{2}(3-y)^{\beta}.
\end{aligned}
$$

- Spatial domain $\Omega = [0,2] \times [0,2]$ and time interval $[0,T] = [0,1]$.
- The source term and the initial condition are fixed such that the exact solution is known.

Number of iterations

N_1	*GMRES*	P_2	P_{MGM}	P_{MGM} (Galerkin)	*Error*
2^4	37.000	21.000	10.000	10.000	9.3706×10^{-2}
2^5	73.000	18.781	11.000	11.000	2.4747×10^{-2}
2^6	137.000	17.000	11.000	11.000	6.3630×10^{-3}
2^7	251.000	17.000	10.000	10.000	1.6053×10^{-3}

Conclusions

Summarizing

- Symbol based analysis for asymptotic eigenvalue/singular value distribution for variable coefficient FDEs.
- Preconditioning: To preserve the structure can be more useful than to preserve the order of the zero of the symbol.
- Multigrid methods preserve the structure without needing to match the order of the zero of the symbol

Future work

- Alternative discretizations like finite volumes[16]
- Applications in imaging, block problems, etc.

[16] Pan, Ng, Wang, *SISC*, 2016

- M. Donatelli, M. Mazza, S. Serra-Capizzano,
  Spectral analysis and structure preserving preconditioners for fractional diffusion equations,
  J. Comput. Phys., 307 (2016), pp. 262–279.
- M. Dehghan, M. Donatelli, M. Mazza, H. Moghaderi,
  Multigrid preconditioners for two-dimensional space-fractional diffusion equations,
  manuscript (2016).

Thanks!