Spectral analysis and structure preserving preconditioners for Fractional Diffusion Equations

Marco Donatelli · Mariarosa Mazza · Stefano Serra-Capizzano

Department of Science and High Technology, University of Insubria, Italy

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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

- $(x,t) \in (L,R) \times (0,T]$,
- $\alpha \in (1,2)$ is the fractional derivative order,
- $f(x,t)$ is the source term,
- $d_\pm(x,t) \geqslant 0$ are the diffusion coefficients,
- $\frac{\partial^\alpha u(x,t)}{\partial_\pm x^\alpha}$ are the left-handed $(+)$ and the right-handed $(-)$ fractional derivatives,

and with the following initial-boundary conditions

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

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

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

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

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

with the formal notation $\begin{pmatrix} \alpha \\ 0 \end{pmatrix} = 1.$

A discretization

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

$$x_i = L + i\Delta x, \quad \Delta x = \frac{(R-L)}{N+1}, \quad i = 0, \dots, N+1,$$
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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

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

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

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

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- $D_\pm^{(m)} = \mathrm{diag}(d_{\pm,1}^{(m)}, \ldots, d_{\pm,N}^{(m)})$ with $d_{\pm,i}^{(m)} := d_\pm(x_i, t_m)$,

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- $\nu_{M,N} = \frac{\Delta x^\alpha}{\Delta t}$,
- $f^{(m)} = [f_1^{(m)}, \ldots, f_N^{(m)}]^T$ with $f_i^{(m)} := f(x_i, t_m)$,
- $u^{(m)} = [u_1^{(m)}, \ldots, u_N^{(m)}]^T$ with $u_i^{(m)} \approx u(x_i, t_m)$.

Preliminaries: symbol

Def1 Let $f \in L^1(-\pi, \pi]$ and let $\{f_j\}_{j\in\mathbb{Z}}$ the sequence of its Fourier coefficients defined as

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

Then the Toeplitz sequence $\{T_n(f)\}_{n\in\mathbb{N}}$ with

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

is called the family of Toeplitz matrices generated by f, which in turn is called the symbol $\{T_n(f)\}_{n\in\mathbb{N}}$.

Preliminaries: spectral distribution

Def2 Let $f : G \to \mathbb{C}$ be a measurable function, defined on a measurable set $G \subset \mathbb{R}^k$ with $k \geqslant 1$, $0 < m_k(G) < \infty$. Let $\{A_N\}$ be a sequence of matrices of size N with eigenvalues $\lambda_j(A_N)$, $j = 1, \dots, N$

- $\{A_N\}$ is distributed as the pair (f, G) in the sense of the eigenvalues, in symbols

$$\{A_N\} \sim_\lambda (f, G),$$

if the following limit relation holds for all $F \in \mathcal{C}_0(\mathbb{C})$:

$$\lim_{N\to\infty} \frac{1}{N} \sum_{j=1}^{N} F(\lambda_j(A_N)) = \frac{1}{m_k(G)} \int_G F(f(t))dt.$$

- The definition of distribution in the sense of the singular values is obtained replacing $\lambda_j \to \sigma_j$, $f(t) \to |f(t)|$, $\mathcal{C}_0(\mathbb{C}) \to \mathcal{C}_0(\mathbb{R}_0^+)$.

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

Recall the coefficient matrix

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

Note: In the constant coefficient case $D_{\pm}^{(m)} = d_{\pm} \cdot I$, $d_{\pm} > 0$, then $\left\{\mathcal{M}_{\alpha,N}^{(m)}\right\}_{N\in\mathbb{N}}$ is a sequence of Toeplitz matrices.

Res1 The symbol associated to the matrix-sequence $\{T_{\alpha,N}\}_{N\in\mathbb{N}}$ is given by

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

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Res2 The sequence of symbols associated to $\left\{\mathcal{M}_{\alpha,N}^{(m)}\right\}_{N\in\mathbb{N}}$ is $\{\varphi_{\alpha,N}\}_{N\in\mathbb{N}}$, with

$$\varphi_{\alpha,N}(\theta) = \nu_{M,N} + d_+ f_\alpha(\theta) + d_- f_\alpha(-\theta).$$

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Res3 Let us assume that $\nu_{M,N} = o(1)$. Given the matrix-sequence $\left\{\mathcal{M}_{\alpha,N}^{(m)}\right\}_{N\in\mathbb{N}}$, we have

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

where $p_{\alpha}(\theta) = f_{\alpha}(\theta) + f_{\alpha}(-\theta) = f_{\alpha}(\theta) + \overline{f_{\alpha}(\theta)}$ is a real-valued continuous function.

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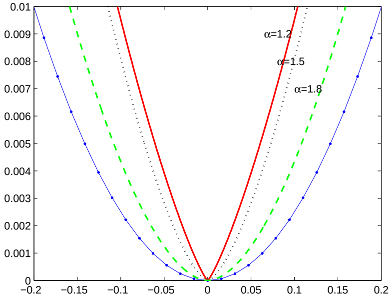
Zero of the symbols $p_\alpha(\theta)$

Res5 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 $p_1(\theta) = \ell(\theta) = \frac{1}{2} p_2(\theta)$.

Preliminaries: GLT sequences

Tool for the variable coefficients case: Generalized Locally Toeplitz (GLT) [3,4] (see Serra-Capizzano's talk Thu 17).

Properties

GLT1 Each GLT sequence has a symbol f in the sense of the singular values over a domain $G = [0,1] \times [-\pi, \pi]$: if the sequence is Hermitian, then the distribution also holds in the eigenvalue sense.

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GLT3 Every Toeplitz sequence with symbol f is a GLT sequence with the same symbol. Every sequence of diagonal matrices $\mathrm{diag}(a(j/N))$ where N is the size of the matrix and a is Riemann integrable over $[0,1]$ is a GLT sequence with symbol a.

[3] Serra-Capizzano, *LAA* 2003
[4] Serra-Capizzano, *LAA* 2006

Preliminaries: GLT sequences

Tool for the variable coefficients case: Generalized Locally Toeplitz (GLT) [3,4] (see Serra-Capizzano's talk Thu 17).

Properties

GLT1 Each GLT sequence has a symbol f in the sense of the singular values over a domain $G = [0, 1] \times [-\pi, \pi]$: if the sequence is Hermitian, then the distribution also holds in the eigenvalue sense.

GLT2 The GLT class is a $*$-algebra. The symbol of linear combinations, products, inversions, conjugations of GLT sequences is obtained by following the same algebraic manipulations on the symbols of the involved GLT sequences.

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

Recall the coefficient matrix

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

Let us assume that $\nu_{M,N} = o(1)$ and that, fixed t_m, $d_{\pm}(x) := d_{\pm}(x, t_m)$ are Riemann integrable over $[L, R]$.

Res4 The matrix sequence $\left\{\mathcal{M}_{\alpha,N}^{(m)}\right\}_{N\in\mathbb{N}}$ is a GLT sequence with symbol

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

and

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

If $d_{+}(x) = d_{-}(x)$, we also have

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

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CGNR with circulant preconditioner and MGM method

Meth1 Conjugate Gradient for Normal Residual (CGNR) with the circulant preconditioner

$$S_N^{(m)} = \nu_{M,N} I + \bar{d}_+^{(m)} s(T_{\alpha,N}) + \bar{d}_-^{(m)} s(T_{\alpha,N})^T,$$

with $\bar{d}_\pm^{(m)} = \frac{1}{N}\sum_{i=1}^{N} d_{\pm,i}^{(m)}$ and $s(T_{\alpha,N})$ the Strang circulant preconditoner.
Superlinearly convergence in the constant coefficients case[5].
An improvement of the circulant preconditioner has been defined in[6].

Meth2 Multigrid method (MGM) with damped-Jacobi as smoother and classical linear interpolation. Optimal convergence of the two-grid in the constant and equal coefficients case[7].

[5] Lei, Sun, *J. Comput. Phys.*, 2013
[6] Pan et al. *SISC*, 2014
[7] Pang, Sun, *J. Comput. Phys.*, 2012

Bad news for the circulant preconditioner

- When $\nu_{M,N} = o(1)$, $\left\{(S_N^{(m)})^{-1}\mathcal{M}_{\alpha,N}^{(m)}\right\}$ is a GLT sequence such that

$$\left\{(S_N^{(m)})^{-1}\mathcal{M}_{\alpha,N}^{(m)}\right\} \sim_\sigma \left(\frac{h_\alpha(x,\theta)}{g_\alpha(\theta)}, [L,R]\times[-\pi,\pi]\right)$$

where $g_\alpha(\theta) = \bar{d}_+^{(m)} f_\alpha(\theta) + \bar{d}_-^{(m)} f_\alpha(-\theta)$. Whenever the diffusion coefficients are nonconstant functions, the preconditioned sequence **CANNOT** be clustered at one, since the function $h_\alpha(x,\theta)/g(\theta)$ is a nontrivial function depending on the variable x.

- Circulant preconditioner **CANNOT** give a proper clustering in the multidimensional problems also in the constant coefficient setting due to the negative results in [8].

[8] Serra-Capizzano, Tyrtyshnikov, *SIMAX*, 1999

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MGM as a valid alternative

Multigrid for 1D constant coefficients FDE was proposed in[7]

- Jacobi smoother and linear interpolation projector.
- The two grid convergence analysis agrees with results for Toeplitz matrices in[9,10].
- 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.

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

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

V-cycle and variable coefficients

- Constant case Given a sequence of Toeplitz matrices $\{A_N\}_{N\in\mathbb{N}}$ with a nonnegative symbol f, the V-cycle optimality requires[11]

$$\limsup_{\theta\to 0} \frac{2+2\cos(\theta+\pi)}{f(\theta)} = c < \infty.$$

  Under the assumption $\nu_{M,N} = o(1)$ and $d_\pm(x,t) = d > 0$, the symbol of the Toeplitz sequence $\left\{\mathcal{M}_{\alpha,N}^{(m)}\right\}_{N\in\mathbb{N}}$ is $f(\theta) = d \cdot p_\alpha(\theta)$ and it satisfies this condition with $c = 0$.
- Nonconstant case When d_+ and d_- are uniformly bounded and positive the optimality of the TGM can be proved like in[12] for PDE.
- Similar results hold in the multidimensional case too, according to[12,13].

[11] Aricò, et all. *SIMAX*, 2004
[12] Serra-Capizzano, *Numer. Math.*, 2002

[13] Aricò, Donatelli, *Numer. Math.*, 2007

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Structure preserving preconditioners for CGNR and GMRES

Why preserving the structure?

- overcome negative results in the multidimensional case;
- have a preconditioned linear system with a well-conditioned matrix of the eigenvectors (useful for GMRES).

1. First preconditioner

$$P_{1,N}^{(m)} = \nu_{M,N} I + D_+^{(m)} B_N + D_-^{(m)} B_N^T,$$

where $B_N = \mathrm{tridiag}_N(0, 1, -1)$ is an approximation of the first derivative operator.

2. Second preconditioner

$$P_{2,N}^{(m)} = \nu_{M,N} I + D_+^{(m)} L_N + D_-^{(m)} L_N^T,$$

where $L_N = \mathrm{tridiag}_N(-1, 2, -1)$ is the Laplacian matrix.

Structure preserving preconditioners for CGNR and GMRES

Computational cost: $P_{1,N}^{(m)}$, $P_{2,N}^{(m)}$ tridiagonal $\rightarrow O(N)$ operations for the associated system $\rightarrow O(N \log N)$ operations for preconditioned Krylov method.

Spectral properties: $P_{1,N}^{(m)}$ and $P_{2,N}^{(m)}$ cannot provide a clustering of the singular values or of the eigenvalues of the preconditioned linear system.

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- The condition number of the preconditioned matrix $P_{2,N}^{(m)} \mathcal{M}_{\alpha,N}^{(m)}$ is asymptotical to $N^{|\alpha-2|}$, with $|\alpha - 2| < 1$ [9]

[9] Serra S., *Calcolo*, 1995

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[9] Serra S., *Calcolo*, 1995

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  effectiveness of the preconditioner $P_{2,N}^{(m)}$ when α is close to 2.

[9] Serra S., *Calcolo*, 1995

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

Numerical results

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

$$\nu_{M,N} = \frac{\Delta x^{\alpha}}{\Delta t} = \Delta x^{\alpha-1}$$

which, being $0 < \alpha - 1 < 1$, tends to zero as N tends to ∞.

- 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.
- Stopping criteria $\|r^k\|/\|r^0\| < 10^{-7}$.

Example 1

- Consider a FDE problem with nonconstant diffusion coefficients

$$d_+(x,t) = \Gamma(3-\alpha)x^{\alpha}, \quad d_-(x,t) = \Gamma(3-\alpha)(2-x)^{\alpha},$$

on the spatial domain $[L, R] = [0, 2]$ and time interval $[0, T] = [0, 1]$.

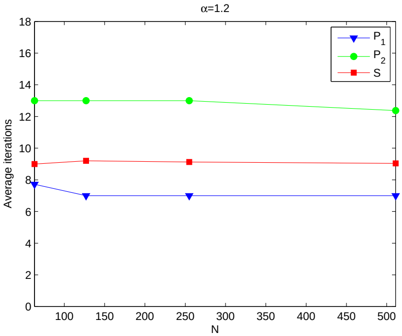
- The source term and the initial condition are fixed such that the exact solution is known.

Number of iterations

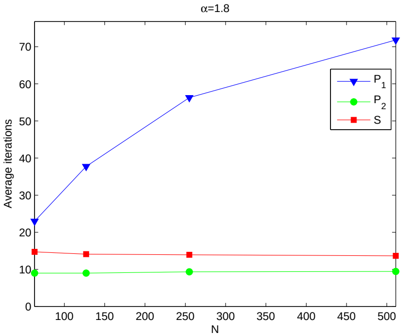
α	$N+1$	P_1		P_2		S	
		CGNR	GMRES	CGNR	GMRES	CGNR	GMRES
1.2	2^6	7.7	8.0	13.0	9.0	9.0	13.0
	2^7	8.0	8.0	13.0	10.0	9.2	14.0
	2^8	7.0	7.0	13.0	10.0	9.1	13.0
	2^9	7.0	7.0	12.4	10.0	9.0	12.0
1.5	2^6	8.0	16.0	12.0	8.0	10.9	12.0
	2^7	18.3	20.0	13.2	9.0	10.7	12.0
	2^8	20.3	24.0	13.9	9.0	11.0	12.0
	2^9	22.4	26.0	14.3	10.0	10.6	12.0
1.8	2^6	9.9	14.6	5.1	4.9	8.4	8.0
	2^7	37.8	40.0	9.0	6.0	14.1	9.0
	2^8	56.3	61.0	9.4	7.0	14.0	9.0
	2^9	71.8	88.0	9.5	7.0	13.7	9.0

CGNR: Average number of iterations varying N

P_1 blue, P_2 green, S red.



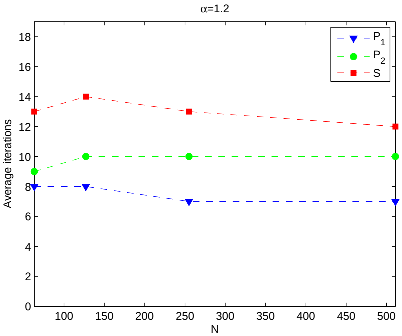
$\alpha = 1.2$



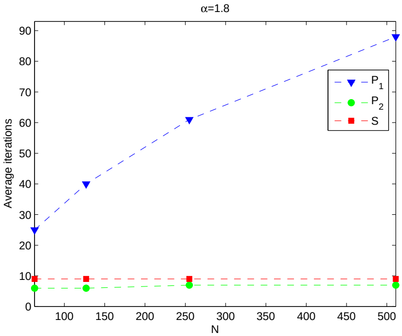
$\alpha = 1.8$

GMRES: Average number of iterations varying N

P_1 blue, P_2 green, S red.



$\alpha = 1.2$



$\alpha = 1.8$

Anomalous diffusive process of a Gaussian pulse

$$\begin{cases} \frac{\partial u(x,t)}{\partial t} = d_+(x,t)\frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha} + d_-(x,t)\frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha} + f(x,t), & (x,t) \in (0,2)\times(0,1], \\ u(0,t) = u(2,t) = 0, & t \in [0,1], \\ u(x,0) = u_0(x), & x \in [0,2]. \end{cases}$$

- diffusion coefficients:

$$d_+(x,t) = 0.1(1 + x^2 + t^2), \quad d_-(x,t) = 0.1(1 + (2-x)^2 + t^2)$$

- source term $\Longrightarrow \quad f(x,t) = 0$
- initial condition $\Longrightarrow \quad u_0(x) = \mathrm{e}^{-\frac{(x-x_c)^2}{2\sigma^2}}$
  with $x_c = 1.2$ and $\sigma = 0.08$

Number of iterations

α	$N+1$	P_1		P_2		S	
		CGNR	GMRES	CGNR	GMRES	CGNR	GMRES
1.2	2^6	5.1	5.0	7.3	6.6	6.8	7.6
	2^7	5.0	5.0	7.0	5.1	6.1	7.0
	2^8	5.0	4.8	6.1	4.1	6.0	7.0
	2^9	4.0	4.0	6.0	3.4	6.0	6.9
1.5	2^6	7.1	8.8	7.0	5.6	7.2	8.4
	2^7	6.8	9.2	7.0	5.1	7.1	8.8
	2^8	6.2	9.2	7.0	5.0	7.0	8.8
	2^9	6.0	9.4	6.5	5.0	7.0	8.7
1.8	2^6	9.9	14.6	5.1	4.9	8.4	8.0
	2^7	10.7	18.7	5.1	5.0	9.2	8.0
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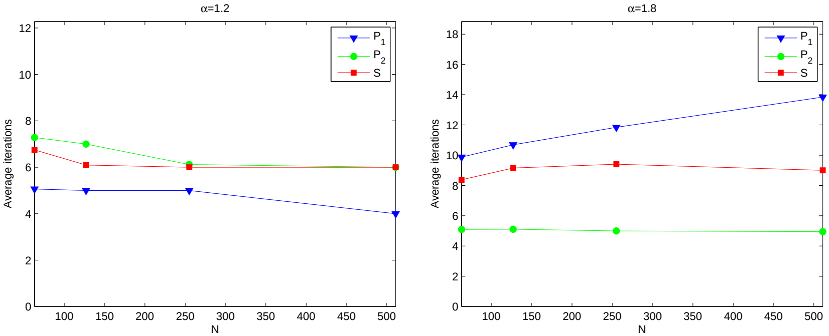

$\alpha = 1.2$ $\alpha = 1.8$

GMRES: Average number of iterations varying N

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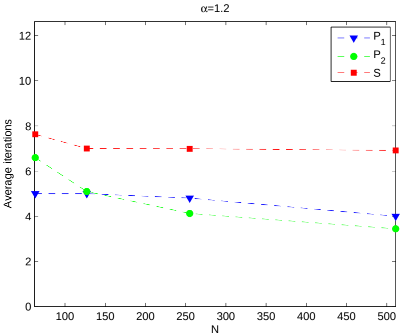
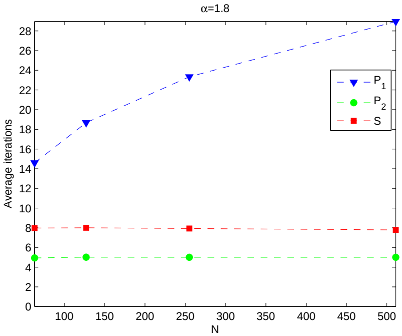


$\alpha = 1.2$



$\alpha = 1.8$

Conclusions

Summirizing

- Asymptotic eigenvalue/singular value distribution for variable coefficient FDEs.
- Analysis of known methods of preconditioned Krylov and multigrid methods, with both positive and negative results.
- Two new tridiagonal structure preserving preconditioners.
- The preconditioner has to match exactly the order α of the zero, while the projector in multigrid need only a zero at π of order not lower than α.

Future work

Spectral analysis, preconditioning and multigrid methods for

- Multidimensional FDEs
- Alternative discretization formulations

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.

Thanks!