Approximated infinite dimensional operators and their Spectral Analysis: the GLT analysis

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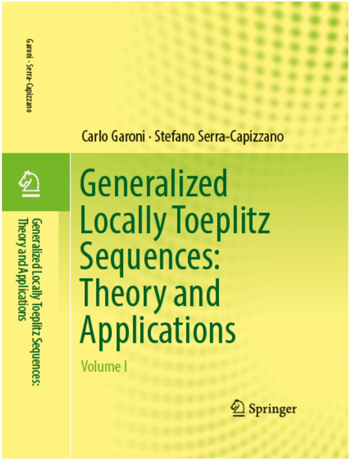
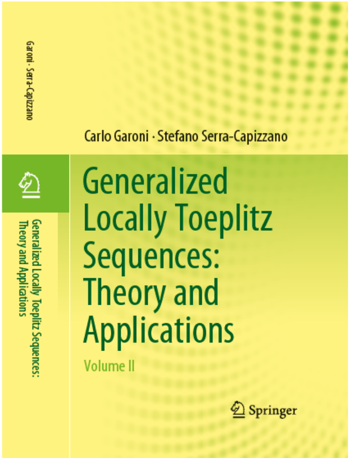
GLT Books: Vol. I ('17), II ('18), III, IV, V long BIT/ETNA papers ('20-'22), VI in preparation)





From continuous to discrete

A continuous infinite-dimensional problem (PDEs, FDEs, IDEs etc) is transformed, via a suitable numerical approximation, into a linear (nonlinear) system of algebraic equations

- Structure inherited from the continuous counterpart
- Large dimensions (e.g. 10^p, $p \geq 10$)
- Spectral features described via a proper Symbol

Goal: solving the resulting linear system by **Optimal Methods** (operation count to obtain the solution of the same order of the matrix-vector multiplication)
Goal: understanding the spectral properties of the resulting matrices (Weyl formulas: **from discrete to continuous**; information for Engineers)

From continuous to discrete

$$\boxed{\text{Linear PDE/FDE/IDE } \mathscr{L}u = g}$$

$$\Downarrow$$

$$\boxed{\text{Linear Numerical Method} \to L_n\mathbf{u}_n = \mathbf{g}_n}$$

- $\dim(L_n) \to \infty$ as $n \to \infty$
- $\{L_n\}$ has an asymptotic spectral distribution described by a spectral/sv symbol

$$\boxed{\text{GLT sequences} = \text{a tool for computing spectral/sv symbols}}$$

$$\boxed{\text{GLT sequences} = \text{a tool for designing fast numer. methods}}$$

$$\boxed{\{L_n\} \text{ is usually a GLT sequence}}$$

In the discrete case

- Large dimensions imply that direct solvers (Gaussian Elimination etc.) have to be avoided
- Iterative solvers: A) operation count per iteration of the same order of the matrix-vector multiplication B) the method is Optimal if the number of iterations $\leq c(\epsilon)$, with ϵ desired precision.

Requirement B) depends on the spectrum of the involved matrices: it depends especially on the possibility of approximating the coefficient matrix in the ill-conditioned subspaces (i.e. associated to the eigenvectors with small eigenvalues).

$$\Downarrow$$

For large classes of matrices coming from continuous problems, **the knowledge of the spectrum** is often compactly represented in a function, called the **symbol**, the GLT symbol: a wide generalization of the (local) Fourier Analysis, see e.g. T.Chan, H.Elman, SIREV 1989

Main items

Symbol for matrix sequences

1. Toeplitz, Diagonal structures and symbol
2. The GLT algebra and the notion of symbol
3. Approximation of Differential Operators

Examples + (preconditioning, multigrid)

4. FEM of degree p in d dimensions
5. IgA of degree p in d dimensions
6. Approximation Q2Q1 of the Linear Elasticity
7. Curl-Div, Curl-Curl, Navier Stokes
8. FDEs and symbol approach
9. The symmetrization (next lecture)

Collaborators

Adriani, Ahmad, Al Aidarous, Barakitis, Barbarino, Beckermann, Benedusi, Bertaccini, Bianchi, Bolten, Böttcher, R. Chan, Donatelli, Dorostkar, Dravins, Dumbser, Durastante, Ekström, Ferrari Furci, Garoni, Golub, Golinskii, Hon, Hughes, Krause, Kuijlaars, Manni, Mazza, Molteni, Neytcheva, Pelosi, Pennati, Ratnani, Reali, Semplice, Sesana, Speleers, Tablino Possio, Tavelli, Tilli, Tyrtyshnikov, Vassalos.

- In blue consolidated collaborations on the themes of the talk;
- In green recently started collaborations (with the goal of variable-coeff. vector PDEs).

$$\Downarrow$$

Elasticity, Navier-Stokes, MHD, evolution PDEs, FDEs ...

The GLT components I: Toeplitz sequences

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

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

$$T_n(f) = \begin{pmatrix} f_0 & f_{-1} & \cdots & \cdots & f_{-(n-1)} \\ f_1 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & f_{-1} \\ f_{n-1} & \cdots & \cdots & f_1 & f_0 \end{pmatrix}$$

The GLT components I: Toeplitz sequences

$$T_n(2-2\cos(\theta)) = \begin{pmatrix} 2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{pmatrix}$$

Its eigenvalues are a sampling of $f(\theta) = 2 - 2\cos(\theta)$:
$\lambda_j = 2 - 2\cos\left(\frac{j\pi}{n+1}\right)$, $j = 1, \ldots, n$.

In general if f is real-valued a.e. then

$$\{T_n(f)\}_n \sim_\lambda f(\theta)$$

and

$$\{T_n(f)\}_n \sim_\sigma f(\theta).$$

The notions $\sim_{\lambda,\sigma}$ generalize that of sampling: more precise definitions later on.

The GLT components II: diagonal sampling matrices

Let $a : [0,1] \to \mathbb{C}$

$$D_n(a) = \begin{pmatrix} a(\frac{1}{n}) & & & \\ & a(\frac{2}{n}) & & \\ & & \ddots & \\ & & & a(1) \end{pmatrix}$$

The eigenvalues of $D_n(a)$ are clearly the samplings of $a(x)$ on $[0,1]$ and

$\{D_n(a)\}_n \sim_{\lambda,\sigma} a(x)$.

The GLT algebra: Toeplitz + Diagonal

GLT sequences = The algebra of matrix sequences containing $\{D_n(a)\}$, a Riemann integrable, $\{T_n(f)\}$, f Lebesgue integrable, $\{X_n\}$ zero distributed sequences.

GLT 1. If $\{A_n\}_n \sim_{\mathrm{GLT}} \kappa$ then $\{A_n\}_n \sim_\sigma \kappa$. If, moreover, the matrices A_n are Hermitian, then $\{A_n\}_n \sim_\lambda \kappa$.

GLT 2. If $\{A_n\}_n \sim_{\mathrm{GLT}} \kappa$ and $A_n = X_n + Y_n$, where

- $\|X_n\|, \|Y_n\| \leq C$ for some constant C independent of n,
- every X_n is Hermitian,
- $\displaystyle\lim_{n\to\infty} \frac{\|Y_n\|_1}{n} = 0$,

then $\{A_n\}_n \sim_\lambda \kappa$.

GLT 3. We have

- $\{T_n(f)\}_n \sim_{\mathrm{GLT}} \kappa(x,\theta) = f(\theta)$ if $f \in L^1(-\pi,\pi)$,
- $\{D_n(a)\}_n \sim_{\mathrm{GLT}} \kappa(x,\theta) = a(x)$ if $a \in C_{\mathrm{a.e.}}[0,1]$,
- $\{Z_n\}_n \sim_{\mathrm{GLT}} \kappa(x,\theta) = 0$ if and only if $\{Z_n\}_n \sim_\sigma 0$.

GLT 4. If $\{A_n\}_n \sim_{\mathrm{GLT}} \kappa$ then $\{A_n^*\}_n \sim_{\mathrm{GLT}} \overline{\kappa}$.

The GLT algebra: Toeplitz + Diagonal

GLT 5. If $A_n = \alpha_1 A_n^{(1)} + \alpha_2 A_n^{(2)}$, with $\alpha_i \in \mathbb{C}$ and $\{A_n^{(i)}\}_n \sim_{\mathrm{GLT}} \kappa_i$, $i = 1, 2$, then $\{A_n\}_n \sim_{\mathrm{GLT}} \kappa = \alpha_1\kappa_1 + \alpha_2\kappa_2$. If $A_n = A_n^{(1)} A_n^{(2)}$, with $\{A_n^{(i)}\}_n \sim_{\mathrm{GLT}} \kappa_i$, $i = 1, 2$, then $\{A_n\}_n \sim_{\mathrm{GLT}} \kappa = \kappa_1\kappa_2$.

GLT 6. If $\{A_n\}_n \sim_{\mathrm{GLT}} \kappa$ and $\kappa \neq 0$ a.e., then $\{A_n^\dagger\}_n \sim_{\mathrm{GLT}} \kappa^{-1}$.

GLT 7. If $\{A_n\}_n \sim_{\mathrm{GLT}} \kappa$ and each A_n is Hermitian, then $\{f(A_n)\}_n \sim_{\mathrm{GLT}} f(\kappa)$ for every continuous function $f : \mathbb{C} \to \mathbb{C}$.

GLT 8. $\{A_n\}_n \sim_{\mathrm{GLT}} \kappa$ if and only if there exist GLT sequences $\{B_{n,m}\}_n \sim_{\mathrm{GLT}} \kappa_m$ such that $\{B_{n,m}\}_n \xrightarrow{\mathrm{a.c.s.}} \{A_n\}_n$ and $\kappa_m \to \kappa$ in measure over $[0, 1] \times [-\pi, \pi]$.

The GLT idea: Toeplitz + Diagonal

As an example (not academical!)

- $A_n = D_n(a_1)T_n(f_1) + T_n(f_2)X_n + Y_n$, with $\{X_n\}$, $\{Y_n\}$ zero distributed sequences
- $\{A_n\}$ has singular values approximated by an equispaced sampling of $|\psi(x,\theta)|$, $\psi(x,\theta) = a_1(x)f_1(\theta)$
- If $\{A_n\}$ is quasi-Hermitian, then $\{A_n\}$ has eigenvalues approximated by an equispaced sampling of $\psi(x,\theta)$

A GLT example: Toeplitz + Diagonal

$\mathcal{L}_a(u) = -\left(a(x)u'\right)'$ [rod with variable section].

$$K_n = \begin{pmatrix} d_1 & -a_{3/2} & & \\ -a_{3/2} & \ddots & \ddots & \\ & \ddots & \ddots & -a_{n-1/2} \\ & & -a_{n-1/2} & d_n \end{pmatrix},$$

$T_n(2-2\cos(\theta)),\ D_n(a) = \mathrm{diag}(a(jh)),\ d_j = a_{j-1/2} + a_{j+1/2}, \quad h = \dfrac{1}{n+1}.$

Then

$$\begin{aligned} K_n &= D_n(a) T_n(2-2\cos(\theta)) + A_n, \quad \|A_n\| \to 0, \\ \psi(x,\theta) &= a(x)(2-2\cos(\theta)). \end{aligned}$$

The eigenvalues of K_n are a sampling of $\psi(x,\theta)$: **this is a GLT result** using items GLT 3., GLT 5., GLT 1.

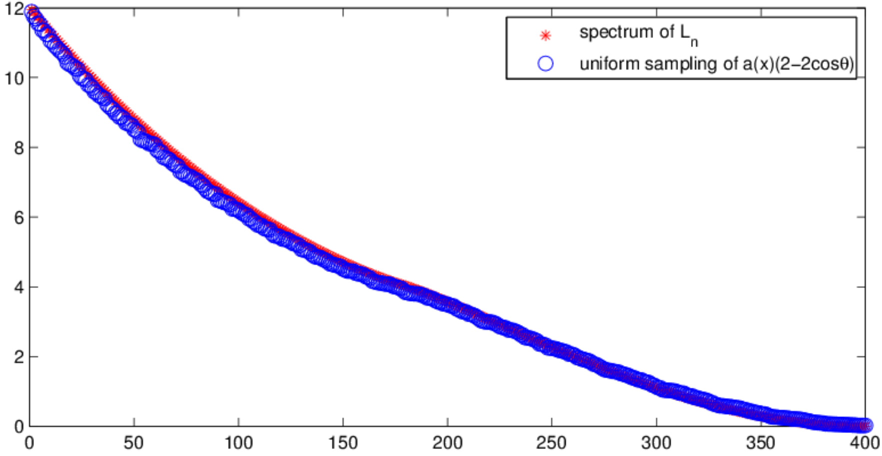


Figure: $a(x) = 2 + \cos(3x)$, $n = 400$. The error on each eigenvalue is of order n^{-1}: can we do better?

Asymptotic Expansion for Banded Symmetric Toeplitz Matrices (....toward matrix-less eigensolvers)

$$\begin{aligned}
\lambda_j(T_n(f)) &= f(\theta_{j,n}) + E_{j,n} \\
&= f(\theta_{j,n}) + \sum_{k=1}^{\alpha} c_k(\theta_{j,n}) h^k + E_{j,n,\alpha} \\
\theta_{j,n} &= \frac{j\pi}{n+1}, \qquad f \text{ monotone}
\end{aligned}$$

1) The same applies to preconditioned structures $\mathcal{P}_n(f,g) = T_n^{-1}(g) T_n(f)$, with g nonnegative not identically zero, and $r = f/g$ (new GLT symbol) monotone;
2) The same applies to structures of the form $M_n^{-1} K_n$, M_n mass matrix, K_n stiffness matrix (also in the variable coefficient case, Ekström's intuition (IgA, FEM)).

Extrapolation Algorithm

We can compute a high precision approximation of $\lambda_j(T_n(f))$ with the following extrapolation algorithm:

- choose m smaller matrices, such that $j_i h_i = jh, i = 1, \ldots, m$;
- compute the eigenvalues $\lambda_{j_1}(T_{n_1}(f)), \ldots, \lambda_{j_m}(T_{n_m}(f))$ using a standard eigensolver;
- compute the errors $E_{j_i,n_i,0} = \lambda_{j_i}(T_{n_i}(f)) - f(\bar{\theta})$ for $i = 1, \ldots, m$, where $\bar{\theta} = \theta_{j,n} = j\pi h$;
- compute $p(h)$, where $p(\cdot)$ is the interpolation polynomial for the data $(h_i, E_{j_i,n_i,0}/h_i),\ i = 1, \ldots, m$, plus $(0, f(\bar{\theta}))$;
- return $f(\bar{\theta}) + hp(h)$.

Numerics

$$f(\theta) = 2 - \cos(\theta) - \cos(3\theta)$$

$$\bar{\theta} = \pi/10$$

m	Error $\left|\lambda_j(T_n(f)) - f(\bar{\theta}) - hp(h)\right|$, $n = 10^6$
1	$7.61 \cdot 10^{-6}$
2	$2.94 \cdot 10^{-7}$
3	$8.76 \cdot 10^{-9}$
4	$2.13 \cdot 10^{-10}$
5	$8.27 \cdot 10^{-12}$

The GLT glasses: a variable-coefficient-operative version of the Local Fourier Analysis

a.1) Local methods (including FDs, FEs, IgA, FVs, VEMs) for approximating PDEs, IEs lead to GLT sequences, possibly after proper permutations

a.2) No limitations on variable coefficients and on domains (grids should have some structure at least asymptotically)

a.3) Information on the symbol leads to information on ill-conditioning, on the size of the ill-conditioned subspaces, on the nature of the ill-conditioned subspaces (low frequencies, high frequencies etc)

The GLT glasses.....

The GLT glasses: a variable-coefficient-operative version of the Local Fourier Analysis

The GLT glasses.....

b.1) We exploit the symbol for understanding the reason of difficulties of known techniques, w.r.t. finess parameters, problem parameters, approximation parameters

b.2) We exploit the symbol for designing new iterative solvers, new preconditioners or smoothers or prolongation operators, aiming at optimality and robustness

Spectral Distribution: the qualitative idea

- $M_m(\mathbb{C})$ complex matrices of order m,
- $\{A_n\}$, $A_n \in M_{d_n}(\mathbb{C})$, $d_n < d_{n+1}$,
- ψ measurable on $D \subset \mathbb{R}^g$, $g \geq 1$,
- ψ being $M_s(\mathbb{C})$-valued, $s \geq 1$,
- $0 < \mu\{D\} < \infty$, $\mu\{\cdot\}$ can be the Lebesgue measure,

$$\{A_n\}_n \sim_\lambda (\psi, D).$$

Informal meaning: $s = 1$. If ψ is continuous, then a suitable ordering of the eigenvalues $\{\lambda_j(A_n)\}$, in correspondence with a equispaced gridding on D, reconstructs approximately the surface $t \to \psi(t)$.
Informal meaning: $s > 1$. If ψ is continuous, then a suitable ordering of the eigenvalues $\{\lambda_j(A_n)\}$, in correspondence with a equispaced gridding on D, reconstructs approximately s surfaces, $t \to \lambda_j(\psi(t))$, $j = 1, \ldots, s$.

Spectral Distribution: the definition

$F \in C_0$ (continuous with compact support):

$$\Sigma_\lambda(F, A_n) = \frac{1}{d_n} \sum_{j=1}^{d_n} F[\lambda_j(A_n)].$$

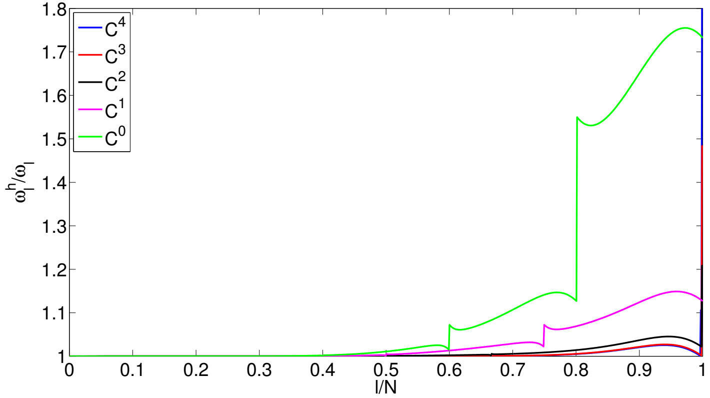
Definition

We write $\{A_n\}_n \sim_\lambda (\psi, D)$ if $\forall F \in C_0$

$$\lim_{n\to\infty} \Sigma_\lambda(F, A_n) = \frac{1}{s\mu\{D\}} \int_D \mathrm{trace}\left(F\left(\psi(t)\right)\right)\, dt.$$

Moreover, we write $\{A_n\}_n \sim_\sigma (\psi, D)$ replacing $\lambda_j(A_n)$ by $\sigma_j(A_n)$ (singular values) in $\Sigma_\sigma(F, A_n)$ in place of $\Sigma_\lambda(F, A_n)$ and replacing $\psi(t)$ by $|\psi(t)|$ in the integral. If $s > 1$ then $|\psi(t)| = \left(\psi^*(t)\psi(t)\right)^{1/2}$.

Comparison IgA-FEM (and furthermore the case of intermediate regularity): $C^0 \rightarrow$FEM$\rightarrow s = p^d$, $C^{p-1} \rightarrow$IgA$\rightarrow s = 1$, $C^k \rightarrow$interm. regularity $\rightarrow s = (p-k)^d$ (figure by A. Reali)



Toeplitz sequences generated by a symbol: $\{T_n(f)\}_n \sim_\lambda (f, I_d)$ if $f = f^*$

- s, d positive integers, $\mathbf{i}^2 = -1$;
- $f \in L^1(I_d, M_s(\mathbb{C}))$, $I_d = (-\pi, \pi)^d$, $j \in \mathbb{Z}^d$;
- $f_j = \frac{1}{(2\pi)^d} \int_{I_d} f(s) e^{-\mathbf{i}js}\, ds$, $f_j \in M_s(\mathbb{C})$.

For $d = 1$ the matrix $T_n(f)$ has size ns:

$$T_n(f) = \begin{pmatrix} f_0 & f_{-1} & \cdots & f_{1-n} \\ f_1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & f_{-1} \\ f_{n-1} & \cdots & f_1 & f_0 \end{pmatrix}.$$

For $d > 1$ we have a recoursive formula.

Toeplitz sequences generated by a symbol: $\{T_n(f)\}_n \sim_\lambda (f, I_d)$ if $f = f^*$

For $d > 1$, the d-level Toeplitz matrix $T_n(f)$ has order Ns, $N = \prod n_j$, $n = (n_1, \ldots, n_d)$, and takes the form

$$T_n(f) = \begin{pmatrix} T_0 & T_{-1} & \cdots & T_{1-n_1} \\ T_1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & T_{-1} \\ T_{n_1-1} & \cdots & T_1 & T_0 \end{pmatrix},$$

T_j being $(d-1)$-level Toeplitz matrix. If $\otimes$ denotes the Kronecker product

$$T_n(f) = \sum_{|j| \le n-1} J_n^{[j]}, \qquad J_n^{[j]} = J_{n_1}^{j_1} \otimes \cdots \otimes J_{n_d}^{j_d} \otimes f_j,$$

with $(J_m^r)_{s,t} = 1$ if $s - t = r$ and 0 otherwise.

FEM: of degree p on a d dimensional domain

We consider the Laplacian over $[0,1]^d$ and we denote by $A_n^{(p)}$ the degree p FEM matrix on quadrilaterals.

- There exists a permutation matrix Π such that

$$\Pi A_n^{(p)} \Pi^T \approx T_n(f);$$

- f is defined over $I_d = (-\pi, \pi)^d$ and Hermitian matrix-valued with size p^d (any comment is redundant!);
- hence, the eigs of $A_n^{(p)}$ are divided into p^d branches (of the same cardinality), each of them represented by a different real-valued eigenvalue of f: $\lambda_1(f) \leq \ldots \leq \lambda_{p^d}$;
- the spreading of the spectrum, measured by the ratio

$$\frac{\max(\lambda_{p^d})}{\max(\lambda_1),}$$

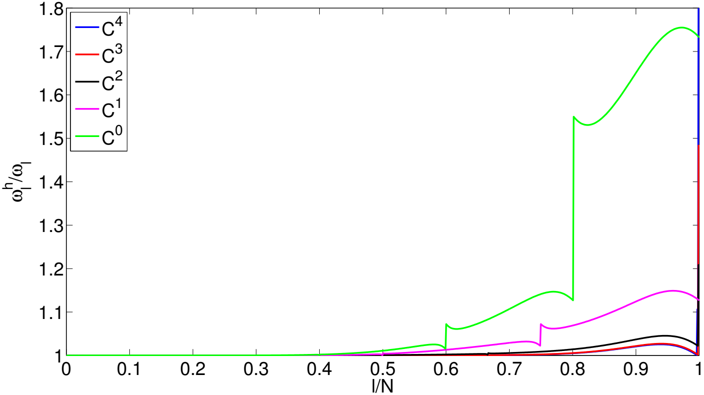
depends on the choice of the basis (Lagrange, integrated Legendre, Bernstein etc); not that of $[M_n^{(p)}]^{-1} A_n^{(p)}$.

IgA: of degree p on a d dimensional domain

We consider the Laplacian over $[0,1]^d$ and we denote by $A_n^{(p)}$ the spline-degree p IgA matrix.

- It holds $A_n^{[p]} \approx T_n(f)$ so that $\{A_n^{(p)}\}_n \sim_\lambda (f, I_d)$, $I_d = (-\pi, \pi)^d$;
- f is defined over $I_d = (-\pi, \pi)^d$, is scalar-valued, nonnegative with a unique zero at zero (as in the FD case: it is somehow the revenge of the smoothness);
- the function f tends exponentially to zero as p in every point of the type $\theta = (\theta_1, \ldots, \theta_d)$ for which $\theta_j = \pi$ for some j;
- the latter property induces a bad conditioning in the high frequency subspace, growing exponentially with p and which is not expected for a differential problem: the knowledge of the symbol is an essential guide for finding the right preconditioner.

Comparison IgA-FEM (and furthermore the case of intermediate regularity): **the picture has a clear interpretation as the revenge of the smoothness**



IgA, degree p, d dimensions: spectral distribution and classical multigrid

Theorem $\boxed{n^{d-2}A_n^{[p]} \approx T_n(f_p)}$ **and hence** $\boxed{\{n^{d-2}A_n^{[p]}\}_n \sim_\lambda (f_p, I_d)}$

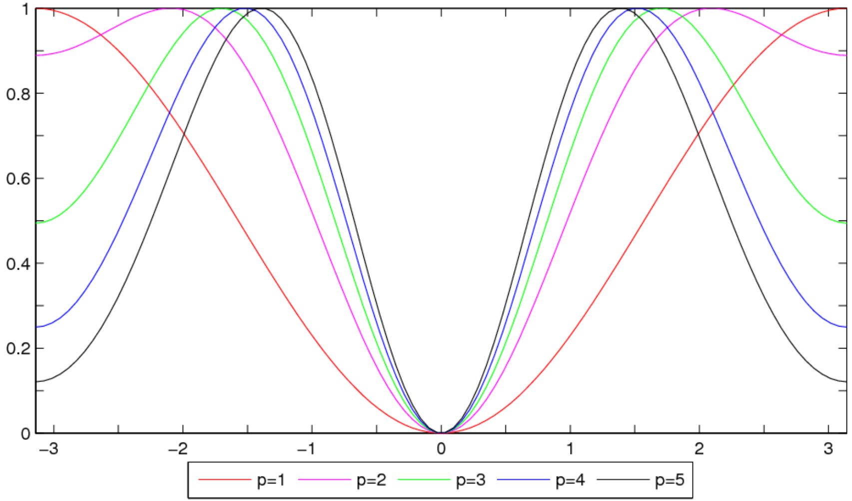
f_p has the expected zero of order 2 at zero, positive elsewhere but it collapses to zero exponentially with p at the boundaries of $I_d = (-\pi, \pi)^d$.

n	$p = 1$	$p = 3$	$p = 5$
16	0.16	0.64	0.96
28	0.17	0.64	0.96
40	0.18	0.64	0.96
52	0.18	0.65	0.96
n	$p = 2$	$p = 4$	$p = 6$
17	0.27	0.88	0.99
29	0.27	0.88	0.99
41	0.29	0.88	0.99
53	0.30	0.88	0.99

Table: spectral radius: standard twogrid, 2D, relaxed GS as smoother

$\approx$ denotes equality up to matrix-sequences with zero symbol.

The graph of f_p



IgA, degree p, d dimensions: structured PCG/PGMRES and multigrid (const. coeff.... but the technique is equally effective for var. coeff. and singular mappings)

We consider the system $nA_n^{[p]}\mathbf{u} = \mathbf{b}$ coming from the IgA approximation of

$$\begin{cases} -\Delta u = 1 & \text{in } (0,1)^3 \\ u = 0 & \text{on } \partial(0,1)^3 \end{cases}$$

For the solution: V-cycle and W-cycle multigrid

n	$p=1$		n	$p=3$		n	$p=5$	
16	10	7	14	7	6	12	8	8
32	11	7	30	8	6	28	8	7
64	12	7	62	9	6	60	9	6

n	$p=2$		n	$p=4$		n	$p=6$	
15	9	8	13	7	6	11	9	9
31	8	7	29	8	6	27	8	6
63	9	7	61	9	6	59	10	6

Table: number of iterations: 3D with structured PCG/PGMRES

IgA, degree p, d dimensions: structured PCG/PGMRES and multigrid

We consider the system $nA_n^{[p]}\mathbf{u} = \mathbf{b}$ coming from the IgA approximation of

$$\begin{cases} -\Delta u = 1 & \text{in } (0,1)^3 \\ u = 0 & \text{on } \partial(0,1)^3 \end{cases}$$

Only one (!) new ingredient in our fast V-cycle

- Standard restriction and prolongation operator;
- Standard smoother (GS) at coarse grids;
- V-cycle with PCG/PGMRES as smoother only at the finest grid;
- Preconditioner chosen by using the information contained in the symbol;
- The preconditioner has a very cheap tensor-banded structure

Variable coefficients: symbol of the IgA matrix-sequences associated to a full elliptic Pb (a GLT sequence)

Full elliptic problem:

$$\begin{cases} -\nabla \cdot K\nabla u + \boldsymbol{\beta} \cdot \nabla u + \gamma u = f & \text{on } \Omega \subset \mathbb{R}^d \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

IgA approximation: take a geometry map $\mathbf{G} : [0,1]^d \to \overline{\Omega}$ to transfer the problem from Ω to $[0,1]^d$; on $[0,1]^d$ use again splines of deg. p.

$$\mathcal{A}_n^{[p]} = \text{resulting IgA approximation matrix}$$

Theorem $\{n^{d-2}\mathcal{A}_n^{[p]}\}_n$ matrix sequence belonging to the GLT algebra

$$\boxed{\{n^{d-2}\mathcal{A}_n^{[p]}\} \sim_\lambda \mathbf{1}\big(|\det(J_{\mathbf{G}}(x_1,\ldots,x_d))|K_{\mathbf{G}}(x_1,\ldots,x_d) \circ H_p(\theta_1,\ldots,\theta_d)\big)\mathbf{1}^T}$$

$$K_{\mathbf{G}} = (J_{\mathbf{G}})^{-1}K(\mathbf{G})(J_{\mathbf{G}})^{-T}, \quad J_{\mathbf{G}} = \text{Jacobian matrix of } \mathbf{G}$$

$H_p =$ symmetric $d \times d$ matrix whose (i,j) entry represents the 'formula' used to approximate $\partial^2/\partial x_i \partial x_j$ **(pull-back idea)**

Further Technical Insights

- The symbol can be recovered in the IgA Collocation/Galerkin setting with variable coefficient PDEs, general physical domain, general geometrical mapping (Bsplines, NURBS).
- The symbol can be recovered in the FEM setting with variable coefficient PDEs, general physical domain, general graded griddings.
- Concerning the numerical methods, the dimensionality d is not an issue and singular mappings are not an issue.
- We are now completing the analysis when the model space is given by GB.

Conclusions

- In the case of constant coefficients PDEs the GLT approach and the Local Fourier Analysis lead to the same conclusions and to the same tools.
- The GLT tool has to be considered as an extension of the Local Fourier Analysis (for variable coefficients, irregular domains etc) and indeed the symbol analysis via GLT is more general and includes also integral problems, preconditioning, involved iteration matrices (PHSS), variable coefficients.
- Future work: Navier-Stokes and other vector problems to be considered, with the idea of using the spectral information and the symbol, in order to obtain faster and more robust (preconditioned) iterative solvers.

Main References

- GLT: Tilli LAA 98, S. LAA 03 e 06 (previous results by Kac, Parter, Widom etc). With Garoni two SPRINGER books
- a.c.s: S. LAA 01, 03, 06 (previous results by Tilli, low norm + low rank by Raymond Chan)
- Spectral Tools (Bottcher, Grudky, Silbermann, Tilli, Tyrtyshnikov, Golinskii, Kuijlaars, S. + coauthors)
- FEM: Beckermann, S. SINUM 07, Garoni, S., Sesana, SIMAX 15
- IgA: Garoni, Manni, Pelosi, S., Speleers NM 14, Donatelli, Garoni, Manni, S., Speleers CMAME 14, CMAME 15, MC 16, MC17
- FDEs: Donatelli, Mazza, S. JCP 16, SISC 18
- Vector Problems: collaborations with Donatelli, Dorostkar, Franck, Garoni, Hughes, Manni, Mazza, Neytcheva, Ratnani, Reali, Sesana, Sonnendrücker, Speleers

Symbol-based NLA for FDEs... and around it

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Fractional Diffusion Equations (FDEs)

We are interested in the following initial-boundary value problem [1]

$$\begin{cases} \frac{\partial u(x,t)}{\partial t} = \int_1^2 \rho(\alpha) \frac{\partial^\alpha u(x,t)}{\partial |x|^\alpha} d\alpha + f(x,t), & (x,t) \in \Omega, \\ u(x,0) = u_0(x), & x \in (a,b), \\ u(a,t) = u(b,t) = 0, & t \in (0,T], \end{cases} \tag{1.1}$$

where

- $\Omega = [a,b] \times [0,T]$,
- $\alpha \in (1,2)$ is the fractional derivative order,
- $f(x,t)$ is the source term,
- $\rho(\alpha)$ is the kernel function and satisfies

$$\rho(\alpha) \geq 0, \;\; 0 < \int_1^2 \rho(\alpha) c(\alpha) < \infty \, , c(\alpha) = -\frac{1}{2\cos(\frac{\alpha\pi}{2})} \, ,$$

- $\frac{\partial^\alpha u(x,t)}{\partial |x|^\alpha}$ is the Riesz fractional derivative and defined as

[1] Abbaszadeh, *Appl. Math. Lett.*, *2019*

Fractional Diffusion Equations (FDEs)

$$\frac{\partial^\alpha u(x,t)}{\partial |x|^\alpha} = c(\alpha)({}_aD_x^\alpha u(x,t) + {}_x D_b^\alpha u(x,t)), \quad c(\alpha) = -\frac{1}{2\cos(\frac{\alpha\pi}{2})} > 0.$$

The left-sided and right-sided Riemann-Liouville (RL) fractional derivatives ${}_aD_x^\alpha u(x,t)$, ${}_xD_b^\alpha u(x,t)$ are in turn defined as

$${}_aD_x^\alpha u(x,t) = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_a^x (x-y)^{1-\alpha} u(y,t)dy,$$

$${}_xD_b^\alpha u(x,t) = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_x^b (y-x)^{1-\alpha} u(y,t)dy,$$

with $\Gamma(\cdot)$ being the gamma function.

Fractional Diffusion Equations (FDEs)

In order to discretize the left and right RL fractional derivatives in space, we exploit the weighted and shifted Grünwald-Letnikov difference scheme given in [3], i.e.,

$$
{}_aD_x^{\alpha} u(x_i,t) = \frac{1}{h^{\alpha}} \sum_{q=0}^{i} \omega_q^{(\alpha)} u(x_{i-q+1},t) + \mathcal{O}(h^2),
$$

$$
{}_xD_b^{\alpha} u(x_i,t) = \frac{1}{h^{\alpha}} \sum_{q=0}^{n-i+1} \omega_q^{(\alpha)} u(x_{i+q-1},t) + \mathcal{O}(h^2),
$$

[11] Hao, Sun, Cao, *J. Comput. Phys., (2015)*

Fractional Diffusion Equations (FDEs)

where

$$\omega_0^{(\alpha)} = \gamma_1(\alpha) g_0^{(\alpha)}, \;\; \omega_1^{(\alpha)} = \gamma_1(\alpha) g_1^{(\alpha)} + \gamma_0(\alpha) g_0^{(\alpha)},$$
$$\omega_k^{(\alpha)} = \gamma_1(\alpha) g_k^{(\alpha)} + \gamma_0(\alpha) g_{k-1}^{(\alpha)} + \gamma_{-1}(\alpha) g_{k-2}^{(\alpha)}, \;\; k \geq 2,$$

in which

$$\gamma_1(\alpha) = \frac{\alpha^2 + 3\alpha + 2}{12}, \, \gamma_0(\alpha) = \frac{4 - \alpha^2}{6}, \, \gamma_{-1}(\alpha) = \frac{\alpha^2 - 3\alpha + 2}{12},$$

$$g_0^{(\alpha)} = 1, \;\; g_{k+1}^{(\alpha)} = \left(1 - \frac{\alpha + 1}{k + 1}\right) g_k^{(\alpha)}, \;\; k \geq 0.$$

A discretization

Let L, m, n be positive integers, $\Delta\alpha = \frac{1}{L}$ be the integration step size, $\Delta t = \frac{T}{m}$ be the time step size, $h = \frac{b-a}{n+1}$ be the spatial width, and consider the following partitions

$$\begin{aligned} \alpha_k &= (k+1/2)\Delta\alpha + 1, \quad k = 0, \cdots, l-1, \\ x_i &= a + ih, \quad i = 0, 1, \cdots, n+1, \\ t_j &= j\Delta t, \qquad j = 0, 1, \cdots, m. \end{aligned}$$

1. discretization in time by an central difference scheme +
2. discretization in space of the fractional derivatives by the weighted and shifted Grünwald-Letnikov difference scheme +
3. quadrature formula for the distributed order

$$=$$

unconditionally stable method[1].

[1] Abbaszadeh, *Appl. Math. Lett., 2019*

Matrix form of the discretized problem

$$(I - A_n)u^{j+1} = (I + A_n)u^j + \Delta t f^{j+\frac{1}{2}}, \tag{1.2}$$

with

$$A_n = \frac{\Delta t \Delta \alpha}{2} \sum_{k=1}^{L} \frac{\rho(\alpha_k)c(\alpha_k)}{h^{\alpha_k}} A_n(\alpha_k), \tag{1.3}$$

- $u^j = (u_1^j, u_2^j, \cdots, u_n^j)^T$ with $u_i^j \approx u(x_i, t_j)$,
- $f^{j+\frac{1}{2}} = (f_1^{j+\frac{1}{2}}, f_2^{j+\frac{1}{2}}, \cdots, f_n^{j+\frac{1}{2}})^T$ with $f_i^{j+\frac{1}{2}} = f(x_i, t_{j+\frac{1}{2}})$,
- I denoting the identity of size n.
- Non-distributed problems: spectral analysis, multigrid, precond. [6, 7, 2] (Barakitis, Donatelli, Ekström, Mazza, Vassalos).

Matrix form of the discretized problem

$$A_n(\alpha_k) = \begin{bmatrix} 2\omega_{\mathbf{1}}^{(\alpha_k)} & \omega_{\mathbf{0}}^{(\alpha_k)} + \omega_{\mathbf{2}}^{(\alpha_k)} & \omega_{\mathbf{3}}^{(\alpha_k)} & \cdots & \omega_{n-\mathbf{1}}^{(\alpha_k)} & \omega_{n}^{(\alpha_k)} \\ \omega_{\mathbf{0}}^{(\alpha_k)} + \omega_{\mathbf{2}}^{(\alpha_k)} & 2\omega_{\mathbf{1}}^{(\alpha_k)} & \omega_{\mathbf{0}}^{(\alpha_k)} + \omega_{\mathbf{2}}^{(\alpha_k)} & \omega_{\mathbf{3}}^{(\alpha_k)} & \cdots & \omega_{n-\mathbf{1}}^{(\alpha_k)} \\ \vdots & \omega_{\mathbf{0}}^{(\alpha_k)} + \omega_{\mathbf{2}}^{(\alpha_k)} & 2\omega_{\mathbf{1}}^{(\alpha_k)} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \omega_{\mathbf{3}}^{(\alpha_k)} \\ \omega_{n-\mathbf{1}}^{(\alpha_k)} & \ddots & \ddots & \ddots & 2\omega_{\mathbf{1}}^{(\alpha_k)} & \omega_{\mathbf{0}}^{(\alpha_k)} + \omega_{\mathbf{2}}^{(\alpha_k)} \\ \omega_{n}^{(\alpha_k)} & \omega_{n-\mathbf{1}}^{(\alpha_k)} & \cdots & \cdots & \omega_{\mathbf{0}}^{(\alpha_k)} + \omega_{\mathbf{2}}^{(\alpha_k)} & 2\omega_{\mathbf{1}}^{(\alpha_k)} \end{bmatrix}.$$

Matrix form of the discretized problem

Equivalently $A_n(\alpha_k) = A_{\alpha_k,n} + A_{\alpha_k,n}^T$, where

$$A_{\alpha_k,n} = \begin{bmatrix} \omega_1^{(\alpha_k)} & \omega_0^{(\alpha_k)} & 0 & \cdots & 0 & 0 \\ \omega_2^{(\alpha_k)} & \omega_1^{(\alpha_k)} & \omega_0^{(\alpha_k)} & \ddots & \ddots & 0 \\ \vdots & \omega_2^{(\alpha_k)} & \omega_1^{(\alpha_k)} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \omega_{n-1}^{(\alpha_k)} & \ddots & \ddots & \ddots & \omega_1^{(\alpha_k)} & \omega_0^{(\alpha_k)} \\ \omega_n^{(\alpha_k)} & \omega_{n-1}^{(\alpha_k)} & \cdots & \cdots & \omega_2^{(\alpha_k)} & \omega_1^{(\alpha_k)} \end{bmatrix}.$$

It is clear that $A_n(\alpha_k)$ is a symmetric Toeplitz matrix. We rewrite the linear system in (1.2) as

$$M_n u^{j+1} = b^j, \tag{1.4}$$

where A_n is as in (1.3) and

$$M_n = I - A_n, \;\; b^j = (I + A_n)\, u^j + \Delta t f^{j+\frac{1}{2}} \,.$$

Preliminaries: generating function vs symbol

Definition

Let $f \in L^1([-\pi,\pi])$ and let $\{f_k\}_{k\in\mathbb{Z}}$ be the sequence of its Fourier coefficients defined as

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

Then the matrix-sequence $\{T_n\}_{n\in\mathbb{N}}$ with $T_n = [f_{i-j}]_{i,j=1}^n$ is called the sequence of Toeplitz matrices generated by f, which in turn is called the generating function of $\{T_n\}_{n\in\mathbb{N}}$ and T_n is denoted by $T_n(f)$.

Preliminaries: spectral distribution

Definition (of the Spectral Symbol)

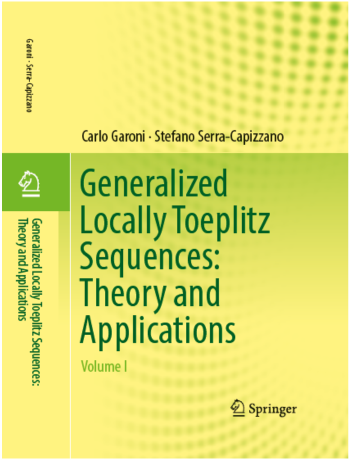
Let $f : [a, b] \to \mathbb{C}$ be a measurable function, defined on $[a, b] \subset \mathbb{R}$, let $\mathcal{C}_0(\mathbb{C})$ be the set of continuous functions with compact support over $\mathbb{C}$ and let $\{\mathcal{A}_n\}_n$ be a sequence of matrices of size n with eigenvalues $\lambda_j(\mathcal{A}_n)$, $j = 1, \ldots, n$. We say that $\{\mathcal{A}_n\}_n$ is distributed as the pair $(f, [a, b])$ in the sense of the eigenvalues, and we write

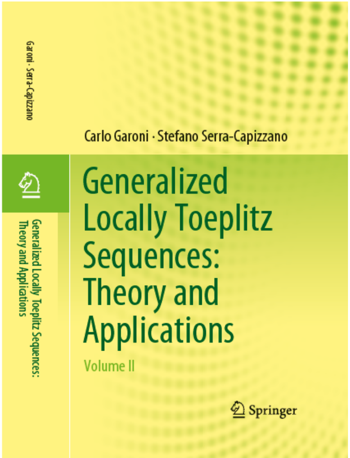
$$\{\mathcal{A}_n\}_n \sim_\lambda (f, [a, b]),$$

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

$$\lim_{n\to\infty} \frac{1}{n} \sum_{j=1}^{n} F(\lambda_j(\mathcal{A}_n)) = \frac{1}{b-a} \int_a^b F(f(t))dt.$$

GLT Books: Vol. I ('17), II ('18), III, IV, V long BIT/ETNA papers ('20-'22), VI in preparation: with Barbarino, Garoni)





Generating function and spectral distribution of $\{A_{\alpha,n}\}_{n\in\mathbb{N}}$

Recall the coefficient matrix

$$A_n = \frac{\Delta t \Delta \alpha}{2} \sum_{k=1}^{L} \frac{\rho(\alpha_k) c(\alpha_k)}{h^{\alpha_k}} A_n(\alpha_k),$$

with $A_n(\alpha_k) = A_{\alpha_k,n} + A_{\alpha_k,n}^T$.

Proposition

Let $\alpha \in (1,2)$. The generating function associated to the Toeplitz matrix-sequence $\{A_{\alpha,n}\}_{n\in\mathbb{N}}$ is given by

$$f_\alpha(\theta) = \sum_{k=-1}^{\infty} \omega_{k+1}^{(\alpha)} e^{\mathbf{i}k\theta} = \left[\frac{8 - 2\alpha^2 + (\alpha^2 + 3\alpha + 2)e^{-\mathbf{i}\theta} + (\alpha^2 - 3\alpha + 2)e^{\mathbf{i}\theta}}{12}\right] \left(1 + e^{\mathbf{i}(\theta+\pi)}\right)^\alpha .$$

Generating function and spectral distribution of $\{A_{\alpha,n}\}_{n\in\mathbb{N}}$

Corollary

Let $\alpha \in (1,2)$. The generating function associated to the Toeplitz matrix-sequence $\{A_n(\alpha) = A_{\alpha,n} + A_{\alpha,n}^T\}_{n\in\mathbb{N}}$ is given by

$$g_\alpha(\theta) = f_\alpha(\theta) + f_\alpha(-\theta)\,.$$

Corollary

Let A_n be the matrix defined in (1.3) and assume that $h^{\Delta\alpha} = o(1)$. Then,

$$\left\{\frac{h^{\alpha_L}}{\Delta t \Delta\alpha} A_n\right\}_{n\in\mathbb{N}} \sim_\lambda \left(c_L\, g_{\alpha_L}(\theta),\, [0,\pi]\right), \quad \textit{where} \quad c_L = \frac{\rho(\alpha_L)c(\alpha_L)}{2}.$$

Symbol and spectral distribution of $\{A_{\alpha,n}\}_{n\in\mathbb{N}}$

Similarly, for the matrix M_n, we prove the following spectral result.

Corollary

For the matrix M_n defined as in (1.4), when $h^{\alpha_L} = o(\Delta t \Delta\alpha)$ and $h^{\Delta\alpha} = o(1)$ it holds

$$\left\{ \frac{h^{\alpha_L}}{\Delta t \Delta \alpha} M_n \right\}_{n\in\mathbb{N}} \sim_\lambda \left(-c_L\, g_{\alpha_L}(\theta),\, [0,\pi] \right), \quad \textit{where} \quad c_L = \frac{\rho(\alpha_L) c(\alpha_L)}{2}.$$

Conditioning and extremal spectral behavior in [4,5,13].

[4] Bogoya, Grudsy, Mazza, SSC, *LAMA*, 2023; [5] Bogoya, Mazza, SSC, Tablino-Possio *BIT*, 2022; [13] Mazza, SSC, Usman, *ETNA*, 2021

Conjugate gradient method

Due to the symmetric positive definite nature of the coefficient matrices, we opt for the preconditioned conjugate gradient (PCG) method and we compare the performances of our proposal with a Strang circulant alternative given in literature [12]. We propose the following two preconditioners (see also [2, 6, 7])

- Laplacian style preconditioner,
- generic τ-preconditioner.

[2] Barakitis, Ekström, Vassalos, *NLAA*, (2022); [6,7] Donatelli, Mazza, Serra-Capizzano, *JCP*, (2016), *SISC*, (2018), [12] Huang, Fang, Sun, Zhang, *LAMA*, 2020

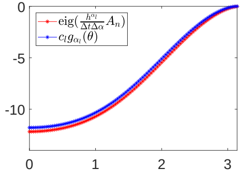
Numerical Example

Under mild conditions on $h^{\alpha_L}, \Delta t, \Delta\alpha$, we prove

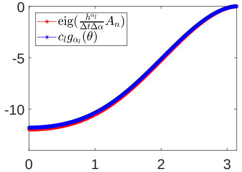
$$\{A_n(\alpha_L)\}_{n\in\mathbb{N}} \sim_\lambda (g_{\alpha_L}(\theta),\, [0,\pi]) \ ,$$

$$\left\{\frac{h^{\alpha_L}}{\Delta t \Delta\alpha} A_n\right\}_{n\in\mathbb{N}} \sim_\lambda (c_L\, g_{\alpha_L}(\theta),\, [0,\pi])\,, \text{ where } c_L = \frac{\rho(\alpha_L)c(\alpha_L)}{2}.$$

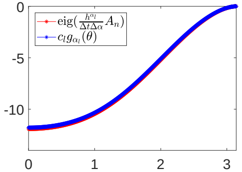
Numerical Example



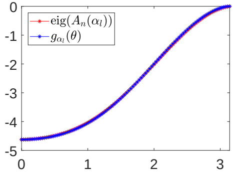
(a) $n = 100$



(b) $n = 500$



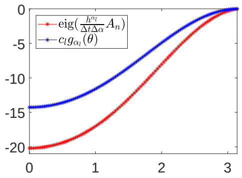
(c) $n = 1000$



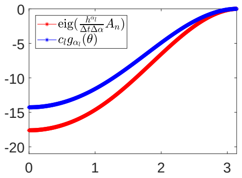
(d) $n = 100$

Figure: (a)–(c) Comparison between the symbol $c_L g_{\alpha_L}(\theta)$ and eig($\frac{h^{\alpha_L}}{\Delta t \Delta \alpha} A_n$) for $L = 2$ and $n = 100, 500, 1000$. (d) Comparison between the symbol $g_{\alpha_L}(\theta)$ and eig($A_n(\alpha_L)$) for $L = 2$ and $n = 100$.

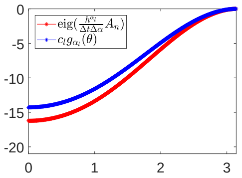
Numerical Example



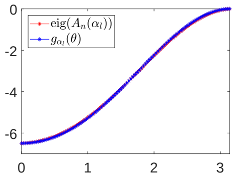
(a) $n = 100$



(b) $n = 1000$



(c) $n = 10000$



(d) $n = 100$

Figure: (a)–(c) Comparison between the symbol $c_L g_{\alpha_L}(\theta)$ and eig($\frac{h^{\alpha_L}}{\Delta t \Delta\alpha} A_n$) for $L = 5$, and $n = 100, 1000, 10000$. (d) Comparison between the $g_{\alpha_L}(\theta)$ and eig($A_n(\alpha_L)$) for $L = 5$ and $n = 100$.

Numerical Example

We now discuss the performances of the PCG method when applied to the following example taken from [12]: assume that in problem equation (1.1) we set

$$\begin{aligned} u(x,0) &= x^2(1-x)^2, \;\; \rho(\alpha) = -2\Gamma(5-\alpha)\cos\left(\frac{\alpha\pi}{2}\right), \\ f(x,t) &= e^t x^2(1-x)^2 - \int_1^2 \rho(\alpha)\frac{\partial^\alpha u(x,t)}{\partial|x|^\alpha}d\alpha \\ &= e^t x^2(1-x)^2 - e^t[f_1(x) + f_1(1-x)], \end{aligned}$$

where

$$\begin{aligned} f_1(x) = \Gamma(5)\frac{1}{\ln x}(x^3 - x^2) - 2\Gamma(4)\left[\frac{1}{\ln x}(3x^2 - 2x) - \frac{1}{(\ln x)^2}(x^2 - x)\right] \\ +\Gamma(3)\frac{1}{\ln x}\left[6x - 2 - \frac{5x}{\ln x} + \frac{3}{\ln x} + \frac{2x}{(\ln x)^2} - \frac{2}{(\ln x)^2}\right]. \end{aligned}$$

Numerical Example

The exact solution for this problem is

$$u(x,t) = e^t x^2 (1-x)^2, \text{ and } (x,t) \in [0,1] \times [0,1].$$

As stopping criterion for the PCG method we consider

$$\frac{||r^{(k)}||_2}{||r^{(0)}||_2} < 10^{-8},$$

where $r^{(k)}$ represents the residual vector after k iterations. In all tables, by "Iter" we mean the average number of iterations after 10 time-steps and by "CPU" the corresponding average timings in seconds.

Numerical Example

$n = m$	Strang circulant		τ preconditioner		Laplacian		$E_2(h)$
	Iter	CPU(s)	Iter	CPU(s)	Iter	CPU(s)	
2^4	4.0	0.0000	4.0	0.0003	7.2	0.0001	1.37e-3
2^5	4.0	0.0000	4.0	0.0003	8.1	0.0001	3.49e-4
2^6	4.0	0.0001	4.0	0.0004	7.2	0.0002	8.66e-5
2^7	4.0	0.0003	4.0	0.0007	7.1	0.0006	2.13e-5
2^8	4.0	0.0007	4.0	0.0012	7.1	0.0011	5.23e-6
2^9	4.0	0.0059	4.0	0.0066	7.2	0.0077	1.28e-6
2^{10}	4.0	0.0166	3.8	0.0180	7.3	0.0284	3.15e-7
2^{11}	3.9	0.0608	3.0	0.0484	7.1	0.1067	7.76e-8
2^{12}	3.7	0.2322	3.1	0.1924	7.1	0.4326	1.92e-8

Table: PCG method performances with three different preconditioners. Here $L = 5$.

Numerical Example

$n = m$	Strang circulant		τ preconditioner		Laplacian		$E_2(h)$
	Iter	CPU(s)	Iter	CPU(s)	Iter	CPU(s)	
2^4	4.0	0.0000	4.0	0.0003	7.1	0.0001	1.37e-3
2^5	4.0	0.0000	4.0	0.0003	8.1	0.0001	3.49e-4
2^6	4.0	0.0001	4.0	0.0004	7.1	0.0002	8.66e-5
2^7	4.0	0.0003	4.0	0.0008	7.1	0.0005	2.13e-5
2^8	4.0	0.0006	4.0	0.0013	7.1	0.0008	5.23e-6
2^9	4.0	0.0052	4.0	0.0065	7.1	0.0078	1.28e-6
2^{10}	4.0	0.0168	4.0	0.0189	6.7	0.0271	3.15e-7
2^{11}	4.0	0.0631	3.1	0.0500	6.1	0.0918	7.76e-8
2^{12}	4.0	0.2516	3.1	0.1984	5.1	0.3097	1.92e-8

Table: PCG method performances with three different preconditioners. Here $L = n$.

Conclusions

- Asymptotic eigenvalue/singular value distribution for constant coefficient FDEs.
- Analysis of known preconditioned Krylov methods.
- Two new preconditioning (Laplacian style preconditioning and generic τ-preconditioning).

Further steps

Adaptations of the same strategies work in the more challenging multilevel setting (for 2D or 3D problems, Mazza, SSC, Sormani, 23). More analysis is needed for different versions of the fractional operators such as the tempered derivatives. Furthermore, there are connections with the notions of the Toeplitz and GLT momentary symbols: see Bolten, Ekström, Furci, SSC, *LAA*, 22 and *ETNA*, 23.

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Thank you for your attention (Q/A) ... second part: an example in higher dimensions and with non Cartesian domains.

Algebra preconditionings for 2D Riesz distributed-order space-fractional diffusion equations on convex domains

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Joint work with Mariarosa Mazza and Rosita Luisa Sormani

Overview

1. Matrix sequences
2. Problem setting and discretization
3. GLT Spectral analysis
4. Algebra preconditioning
5. Numerical experiments

Matrix sequences

$\{A_N\}_N$ = Sequence of matrices of increasing dimension as $N \to \infty$.

Spectral symbol of $\{A_N\}_N$ = function F_a such that the eigenvalues of A_N are approximately a uniform sampling of F_a over its domain.

Notation: $\{A_N\}_N \sim_\lambda F_a$

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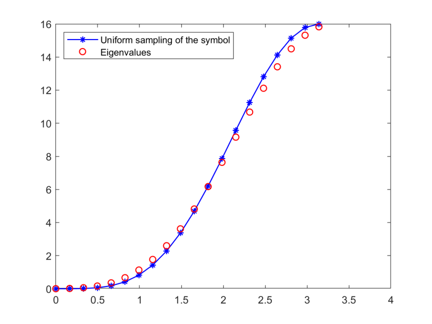
An example:

$$A_N = \text{pentadiag}[1, -4, 6, -4, 1]$$

$$F_a(\theta) = (2 - 2\cos(\theta))^2$$

It holds

$$\{A_N\}_N \sim_\lambda F_a \quad \text{on } [0, \pi]$$



$N = 20$

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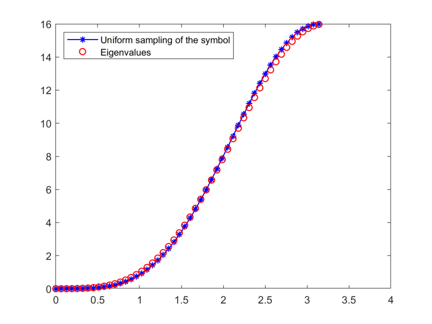

$N = 50$

Spectral symbol

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Spectral symbol of $\{A_N\}_N$ = function F_a such that the eigenvalues of A_N are approximately a uniform sampling of F_a over its domain.

Notation: $\{A_N\}_N \sim_\lambda F_a$

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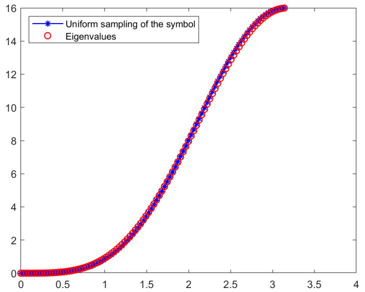

$N = 100$

GLT Algebra Set of matrix sequences closed under linear combinations, product and (pseudo)inversion.

- It contains:
  - Toeplitz sequences with L^1 symbols
  - Diagonal sampling matrices with Riemann integrable symbols
  - Zero-distributed sequences
- Each GLT sequence is equipped with a symbol

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- Each GLT sequence is equipped with a symbol

$$\text{GLT algebra} \longrightarrow \text{Symbols}$$

$$\{A_N\}_N \longrightarrow F_a$$

is an algebra homomorphism

Problem setting and discretization

Consider the 2D distributed order space-fractional diffusion equation

$$\frac{\partial u(x,y,t)}{\partial t} = \int_1^2 \left(\frac{\partial^\alpha u(x,y,t)}{\partial |x|^\alpha} + \frac{\partial^\alpha u(x,y,t)}{\partial |y|^\alpha} \right) \rho(\alpha)\mathrm{d}\alpha + f(u,x,y,t),$$
$$(x,y) \in \Omega,\ t \in [0,T]$$

with initial and boundary conditions

$$\begin{cases} u(x,y,0) = u_0(x,y), & (x,y) \in \Omega, \\ u(x,y,t) = 0, & (x,y) \in \mathbb{R}^2 \backslash \Omega,\ t \in (0,T] \end{cases}$$

where Ω is a convex region

Non-Cartesian domain $\Rightarrow$ Non-Cartesian meshes

- Extra care needed for the boundary
- Difficult to implement
- Linear systems with **hidden structures or unstructured coefficient matrices**

Continuous problem

Non-Cartesian domain $\Rightarrow$ Non-Cartesian meshes

- Extra care needed for the boundary
- Difficult to implement
- Linear systems with **hidden structures or unstructured coefficient matrices**

$$\downarrow$$

Volume-penalization method

1. Embed the domain into a rectangle $[a, b] \times [c, d] = \tilde{\Omega} \supseteq \Omega$
2. Extend the problem to $\tilde{\Omega}$
3. Add a penalization term that dominates on $\tilde{\Omega} \setminus \Omega$, annihilating the solution

Extended continuous problem

$$\frac{\partial u_\eta(x,y,t)}{\partial t} = \int_1^2 \left(\frac{\partial^\alpha u_\eta(x,y,t)}{\partial |x|^\alpha} + \frac{\partial^\alpha u_\eta(x,y,t)}{\partial |y|^\alpha} \right) \rho(\alpha) d\alpha + \tilde{f}(u_\eta, x, y, t)$$
$$- \frac{1 - 1_\Omega(x,y)}{\eta} u_\eta(x,y,t), \qquad (x,y) \in \tilde{\Omega},\ t \in [0,T]$$

with initial and boundary conditions

$$\begin{cases} u_\eta(x,y,0) = \tilde{u}_0(x,y), & (x,y) \in \tilde{\Omega}, \\ u_\eta(x,y,t) = 0, & (x,y) \in \mathbb{R}^2 \backslash \tilde{\Omega},\ t \in (0,T], \end{cases}$$

where

- $\tilde{\Omega} = [a,b] \times [c,d] \supseteq \Omega$
- η is the penalty parameter and $u_\eta \xrightarrow{\eta \to 0^+} u$
- 1_Ω is the characteristic function of Ω
- $\tilde{f}, \tilde{u}_0$ are zero extensions for f, u_0

Cartesian domain $\Rightarrow$ Uniform spatial grids $\{x_i\}_{i=1}^{n_1}$, $\{y_j\}_{j=1}^{n_2}$

- Finite difference methods
- Linear systems with **structured matrices**

Discretization

Cartesian domain $\Rightarrow$ Uniform spatial grids $\{x_i\}_{i=1}^{n_1}$, $\{y_j\}_{j=1}^{n_2}$

- Finite difference methods
- Linear systems with **structured matrices**

Coefficient matrix

$$M_N = L_N + D_N, \qquad M_N \in \mathbb{R}^{N\times N}, N = n_1 n_2$$

- L_N corresponds to the **original problem** and is a 2-level Toeplitz

$$L_N = I_N - I_{n_2} \otimes B^x_{n_1} - B^y_{n_2} \otimes I_{n_1}$$

- D_N corresponds to the added **penalization term** and is diagonal

$$D_N = \mathbf{diag}\left[d_{i,j}\right]_{\substack{i=1,\dots,n_1\\ j=1,\dots,n_2}} \qquad d_{i,j} \neq 0 \iff (x_i, y_j) \in \tilde{\Omega} \setminus \Omega$$

- M_N is symmetric and positive definite

GLT Spectral analysis

Symbol of $\{M_N\}_N$

To compute the symbol of

$$\begin{aligned} M_N &= I_N - I_{n_2} \otimes B^x_{n_1} - B^y_{n_2} \otimes I_{n_1} + D_N \\ &= I_N - A^x_N - A^y_N + D_N \end{aligned}$$

1. Compute F_i, F_{a^x}, F_{a^y}, F_d, symbols of $\{I_N\}_N$, $\{A^x_N\}_N$, $\{A^y_N\}_N$, $\{D_N\}_N$
2. Compute $F_m = F_i - F_{a^x} - F_{a^y} + F_d$, symbol of $\{M_N\}_N$

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2. Compute $F_m = F_i - F_{a^x} - F_{a^y} + F_d$, symbol of $\{M_N\}_N$

Theorem

With suitable hypothesis on the parameters,

$$\{t_x M_N\}_N \sim_\lambda \mathcal{F}_\alpha(\theta_1, \theta_2) + 1_{\tilde{\Omega}\setminus\Omega} C_\eta$$

where $\mathcal{F}_\alpha(\theta_1, \theta_2)$ is defined on $[0, \pi]^2$ and $C_\eta \xrightarrow{\eta \to 0^+} \infty$.

Comparison between the symbol $\mathcal{F}_\alpha(x, y, \theta_1, \theta_2)$ and $\mathrm{eig}(t_x M_N)$

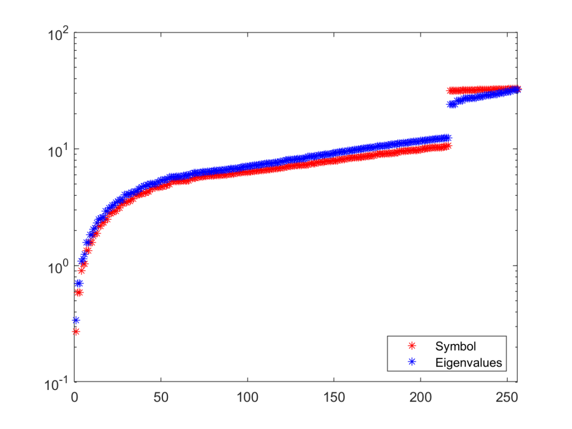

Figure 1: $\eta = 10^{-4}$, $n_1 = n_2 = 2^4$

Symbol of $\{M_N\}_N$

Comparison between the symbol $\mathcal{F}_\alpha(x, y, \theta_1, \theta_2)$ and $\text{eig}(t_x M_N)$

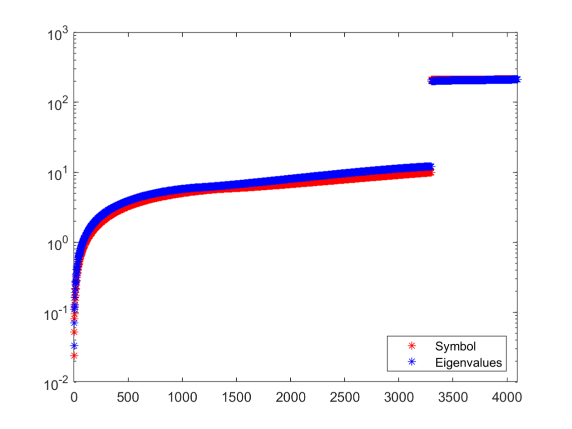

Figure 2: $\eta = 10^{-6}$, $n_1 = n_2 = 2^6$

Algebra preconditioning

Preconditioning proposal 1

$$\mathcal{T}_N = I_N - I_{n_2} \otimes \mathcal{T}(B^x_{n_1}) - \mathcal{T}(B^y_{n_2}) \otimes I_{n_1}$$
$$\mathcal{S}_N = I_N - I_{n_2} \otimes \mathcal{S}(B^x_{n_1}) - \mathcal{S}(B^y_{n_2}) \otimes I_{n_1}$$

with

- $\mathcal{T}(B^x_{n_1})$, $\mathcal{T}(B^y_{n_2})$ τ-preconditioners of $B^x_{n_1}$, $B^y_{n_2}$
- $\mathcal{S}(B^x_{n_1})$, $\mathcal{S}(B^y_{n_2})$ circulant preconditioners of $B^x_{n_1}$, $B^y_{n_2}$

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- $\mathcal{S}(B^x_{n_1}), \mathcal{S}(B^y_{n_2})$ circulant preconditioners of $B^x_{n_1}, B^y_{n_2}$

Theorem

With suitable hypothesis on the parameters,

$$\{t_x \mathcal{T}_N\}_N, \{t_x \mathcal{S}_N\}_N \sim_\lambda \mathcal{F}_\alpha(\theta_1, \theta_2)$$

Preconditioning proposal 2

$$\mathcal{T}_N^{\mathrm{split}} = \mathcal{D}_N(1_\Omega)\mathcal{T}_N + \mathcal{D}_N(1_{\tilde{\Omega}\setminus\Omega})\left(\mathcal{T}_N + \frac{\Delta t}{2\eta} I_N\right)$$
$$\mathcal{S}_N^{\mathrm{split}} = \mathcal{D}_N(1_\Omega)\mathcal{S}_N + \mathcal{D}_N(1_{\tilde{\Omega}\setminus\Omega})\left(\mathcal{S}_N + \frac{\Delta t}{2\eta} I_N\right)$$

based on the alternative splitting for M_N

$$M_N = \mathcal{D}_N(1_\Omega)L_N + \mathcal{D}_N(1_{\tilde{\Omega}\setminus\Omega})\left(L_N + \frac{\Delta t}{2\eta} I_N\right)$$

where $\mathcal{D}_N(1_\Omega) = \mathrm{diag}\left[1_\Omega\left(\frac{i}{n_1+1}, \frac{j}{n_2+1}\right)\right]_{\substack{i=1,\dots,n_1\\ j=1,\dots,n_2}}$

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Theorem

With suitable hypothesis on the parameters,

$$\left\{t_x\mathcal{T}_N^{\mathrm{split}}\right\}_N, \left\{t_x\mathcal{S}_N^{\mathrm{split}}\right\}_N \sim_\lambda \mathcal{F}_\alpha(\theta_1,\theta_2) + 1_{\tilde{\Omega}\setminus\Omega}C_\eta$$

Numerical experiments

τ VS CIRCULANT

$\mathcal{S}_N$, $\mathcal{S}_N^{\text{split}}$

- Worse matching of small eigenvalues

$\mathcal{T}_N$, $\mathcal{T}_N^{\text{split}}$

- Better matching of small eigenvalues

Table 1: $\eta = 10^{-2}$

	PCG			
	$\mathcal{S}_N$		$\mathcal{T}_N$	
$n_1 = n_2$	Iter	CPU	Iter	CPU
2^7	18.90	0.0708	5.10	0.0313
2^8	22.90	0.2479	5.10	0.0983
2^9	29.90	1.9227	5.20	0.4682
2^{10}	35.50	7.6379	5.80	1.9621

τ VS CIRCULANT

$\mathcal{S}_N$, $\mathcal{S}_N^{\text{split}}$	$\mathcal{T}_N$, $\mathcal{T}_N^{\text{split}}$
• Worse matching of small eigenvalues	• Better matching of small eigenvalues

Table 1: $\eta = 10^{-2}$

	GMRES			
	$\mathcal{S}_N^{\text{split}}$		$\mathcal{T}_N^{\text{split}}$	
$n_1 = n_2$	Iter	CPU	Iter	CPU
2^7	18.20	0.1001	6.00	0.0640
2^8	22.60	0.3865	7.00	0.2227
2^9	27.20	1.9674	7.00	0.8897
2^{10}	32.80	9.3339	6.20	3.5411

Non-split VS Split

$\mathcal{S}_N$, $\mathcal{T}_N$

- Symbol does not balance the large outliers due to D_N

$\mathcal{S}_N^{\text{split}}$, $\mathcal{T}_N^{\text{split}}$

- Symbol balances the large outliers due to D_N

Table 2: $\eta = 10^{-3}$

	PCG		GMRES	
	$\mathcal{S}_N$	$\mathcal{T}_N$	$\mathcal{S}_N^{\text{split}}$	$\mathcal{T}_N^{\text{split}}$
$n_1 = n_2$	Iter	Iter	Iter	Iter
2^7	19.00	7.10	17.00	8.00
2^8	24.10	7.00	21.80	8.00
2^9	30.10	7.00	26.90	8.00
2^{10}	43.30	8.10	34.20	7.20

Non-split VS Split

$\mathcal{S}_N, \mathcal{T}_N$

- Symmetric $\Rightarrow$ PCG can be used
- 2 fast transforms less

$\mathcal{S}_N^{\text{split}}, \mathcal{T}_N^{\text{split}}$

- Non-symmetric $\Rightarrow$ Resort to GMRES
- 2 fast transforms more

Table 2: $\eta = 10^{-3}$

	PCG		GMRES	
	$\mathcal{S}_N$	$\mathcal{T}_N$	$\mathcal{S}_N^{\text{split}}$	$\mathcal{T}_N^{\text{split}}$
$n_1 = n_2$	CPU	CPU	CPU	CPU
2^7	0.0689	0.0409	0.0940	0.0808
2^8	0.2527	0.1242	0.3503	0.2581
2^9	1.5727	0.5657	1.9032	0.9314
2^{10}	8.7480	2.5431	9.9982	3.9584

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Thank You
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