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On the extreme eigenvalues and asymptotic conditioning of a class of Toeplitz matrix-sequences arising from fractional problems

Manuel Bogoya ^{a,b}, Sergei Grudsky ^c, Mariarosa Mazza ^b and Stefano Serra-Capizzano ^b

^aDepartamento de Matemáticas, Universidad del Valle, Cali, Colombia; ^bDipartimento di Scienza e Alta Tecnologia, Università dell'Insubria, Como, Italy; ^cDepartamento de Matemáticas, CINVESTAV del I.P.N., Ciudad de Mexico, Mexico

ABSTRACT

The analysis of the spectral features of a Toeplitz matrix-sequence $\{T_n(f)\}_{n \in \mathbb{N}}$, generated by the function $f \in L^1([-\pi, \pi])$, real-valued almost everywhere (a.e.), has been provided in great detail in the last century, as well as the study of the conditioning, when f is nonnegative a.e. Here we consider a novel type of problem arising in the numerical approximation of distributed-order fractional differential equations (FDEs), where the matrices under consideration take the form

$$\begin{aligned} T_n = c_0 T_n(f_0) + c_1 h^h T_n(f_1) + c_2 h^{2h} T_n(f_2) + \dots \\ + c_{n-1} h^{(n-1)h} T_n(f_{n-1}), \end{aligned}$$

c_0, c_1, \dots, c_{n-1} belong to the interval $[c_*, c^*]$ with $c^* \geq c_* > 0$ independent of n , $h = \frac{1}{n}$, $f_j \sim g_j$, and $g_j(\theta) = |\theta|^{2-jh}$ for every $j = 0, \dots, n-1$. For nonnegative functions or sequences, the notation $s(x) \sim t(x)$ means that there exist positive constants c, d , independent of the variable x in the definition domain such that $cs(x) \leq t(x) \leq ds(x)$ for any x . Since the resulting generating function depends on n , the standard theory cannot be applied and the analysis has to be performed using new ideas. Few selected numerical experiments are presented, also in connection with matrices that come from distributed-order FDE problems, and the adherence with the theoretical analysis is discussed, together with open questions and future investigations.

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1. Introduction

In many practical applications, it is required to solve numerically linear systems of Toeplitz kind and of (very) large dimensions, and hence several specialized techniques of iterative type, such as preconditioned Krylov methods and ad hoc multigrid procedures have been

CONTACT Mariarosa Mazza  mariarosa.mazza@uninsubria.it Dipartimento di Scienza e Alta Tecnologia, Università dell'Insubria, Via Valleggio 11, 22100 Como, Italy

designed; we refer the interested reader to the books [1,2] and to the references therein. We recall that such types of large Toeplitz linear systems emerge from specific applications involving, e.g., the numerical solution of (integro-) differential equations and problems with Markov chains. On the other hand, quite recently, new examples of real-world problems have emerged and among them we can cite the modelling of anomalous diffusion processes, which naturally lead to the use of fractional differential equations (FDEs). Also, in this case, we encounter Toeplitz structures, which are dense since the fractional operators are inherently nonlocal, and hence new numerical challenges have come into play. In all the considered applications, the sizes of the resulting matrices are large and iterative solvers have to be considered, both for numerical stability and computational issues. The convergence analysis of such iterative procedures can be performed when we know the spectral features of the considered coefficient matrices. This has been done in the recent literature for certain constant-order FDE problems (see, e.g., Refs. [3–5]), by exploiting the well-established analysis of the spectral features of Toeplitz matrix-sequences generated by Lebesgue integrable functions and the more recent Generalized Locally Toeplitz theory [6].

Here we consider a novel type of problem arising in the numerical approximation of distributed-order fractional operators. The latter can be interpreted as a parallel distribution of derivatives of fractional orders, whose most immediate application consists in the physical modelling of systems characterized by a superposition of different processes operating in parallel. As an example, we mention the application of fractional distributed-order operators as a tool for accounting memory effects in composite materials [7] or multi-scale effects [8]. For a detailed review on the topic, we refer the reader to Ref. [9]. The procedure to numerically approximate distributed-order operators is made of two steps: (i) as the distributed-order operator consists of a continuous distribution of fractional order, a numerical integration is used to discretize the distributed-order operator into a multi-term constant-order fractional derivative; (ii) an approximation method has to be used for discretizing each constant-order fractional derivative composing the multi-term derivative.

In this paper, we focus on the case left open in Ref. [10], which arises when the integral partition width used in step (i) is asymptotic to the discretization step adopted in (ii) and where the matrices under consideration take the form

$$\mathcal{T}_n := c_0 T_n(f_0) + c_1 h^h T_n(f_1) + c_2 h^{2h} T_n(f_2) + \dots + c_{n-1} h^{(n-1)h} T_n(f_{n-1}), \quad (1)$$

where $T_n(f_j)$ is the Toeplitz matrix of size n generated by f_j , the constants c_0, c_1, \dots, c_{n-1} belong to the interval $[c_*, c^*]$, $c^* \geq c_* > 0$, and are independent of $n, h := \frac{1}{n}, f_j \geq 0$ a.e. and given $g_j(\theta) := |\theta|^{2-jh}, j = 0, \dots, n-1$ there exist positive constants d_*, d^* independent of j and n , satisfying

$$d_* g_j \leq f_j \leq d^* g_j \text{ a.e., } j = 0, \dots, n-1,$$

(see, e.g., Refs. [10–13] and the references therein). Taking into consideration the linearity of the operators $T_n(\cdot)$, $n \geq 1$, since the resulting generating function

$$F_n(\theta) := \sum_{j=0}^{n-1} c_j h^{jh} f_j(\theta)$$

depends on n , the standard theory cannot be applied in a straightforward manner, and the analysis has to be performed using new ideas. The description and the exploitation of such new ideas is the main topic of this paper.

The organization of the paper is quite simple. In Section 2, we briefly recall some properties of Toeplitz matrices and the linear positive operator $T_n(\cdot)$ that will be used in Section 3 to provide asymptotic estimates for the extreme eigenvalues of T_n in (1). In Section 4, we show and critically discuss few selected numerical examples for illustrating our theoretical findings. Finally, Section 5 is devoted to conclusions and to state few open problems.

2. A few preliminaries

Given a Lebesgue integrable function f defined on $[-\pi, \pi]$, i.e. $f \in L^1([-\pi, \pi])$, and periodically extended to the whole real line, let us consider the Toeplitz matrix $T_n(f)$ of size n generated by f . For any n , the entries of $T_n(f)$ are defined via the Fourier coefficients $\{\alpha_k(f)\}_k$, $k \in \mathbb{Z}$, of f in the sense that

$$(T_n(f))_{s,t} = \alpha_{s-t}(f), \quad s, t \in \{1, \dots, n\},$$

and

$$\alpha_k(f) := \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\theta) e^{-ik\theta} d\theta, \quad k = 0, \pm 1, \pm 2, \dots, \quad i^2 = -1.$$

The function f is called the *generating function* of $T_n(f)$. In the general case, f is complex-valued and $T_n(f)$ is non-Hermitian for all sufficiently large n . However, if f is real-valued a.e., then $T_n(f)$ is Hermitian for all n . Furthermore, when f is real-valued and even a.e., the matrix $T_n(f)$ is (real) symmetric for all n [6].

As it is well known in the literature, the operator $T_n: L^1([-\pi, \pi]) \rightarrow M_n(\mathbb{C})$ is a linear positive operator, briefly LPO, in the sense that:

Linearity: $T_n(\alpha f + \beta g) = \alpha T_n(f) + \beta T_n(g)$, for any constants $\alpha, \beta \in \mathbb{C}$, and any functions $f, g \in L^1([-\pi, \pi])$.

Positivity: $T_n(f)$ is Hermitian nonnegative definite for any size $n \geq 1$ if $f \geq 0$ a.e.

For more details on LPOs, we refer the reader to Ref. [14] and to the beautiful book [15]. Here we just recall that the linearity is a trivial fact coming from the linearity of the Fourier coefficients with respect to their argument f , while the second property is less obvious. In reality, as proven in Ref. [14], the positivity holds even in a stronger sense because $f \geq 0$ a.e. and f not identically zero a.e. imply that $T_n(f)$ is positive definite for any $n \geq 1$: conversely, $f \equiv 0$ a.e. means that $T_n(f)$ is trivially the null matrix of size $n \geq 1$.

Furthermore, it is a simple check to show that linearity and positivity imply monotonicity, and hence from $f \geq g$ a.e. we deduce that $T_n(f) - T_n(g)$ is nonnegative definite and we write $T_n(f) \geq T_n(g)$ (respectively positive definite if $f - g$ is not identically zero a.e. and we write $T_n(f) > T_n(g)$).

We conclude the current section by fixing the notation adopted throughout the paper. Given a square complex matrix $B := (b_{s,t})_{s,t=1}^n$, by $\|B\|_p$ we mean the matrix norm induced

by the vector p -norm, i.e.

$$\|B\|_p := \sup \left\{ \frac{\|Bx\|_p}{\|x\|_p} : x \neq 0 \right\},$$

and precisely $\|B\|_1 = \max_s \sum_t |b_{s,t}|$ and $\|B\|_2 = \sigma_{\max}(B)$, also known as spectral norm. We recall that when B is Hermitian or symmetric we have $\|B\|_2 = \rho(B)$, with $\rho(B)$ being the spectral radius of B and, as a consequence, that $\|B\|_2 \leq \|B\|_1$. Finally, when considering an invertible matrix B , with $\mu_2(B)$ we refer to the spectral condition number, i.e.

$$\mu_2(B) := \|B^{-1}\|_2 \|B\|_2 = \frac{\sigma_{\max}(B)}{\sigma_{\min}(B)}.$$

3. Analysis of the problem

The set of properties introduced in Section 2 allows one to deduce the following general result regarding the considered class of quite involved matrices (1), arising in the numerical approximation of distributed-order FDEs (see Ref. [12]).

Theorem 3.1: *For $j = 0, \dots, n-1$, let f_j be an essentially bounded function defined on $[-\pi, \pi]$ such that there exist positive constants $d_*, d^* > 0$, independent of j and of n , for which*

$$d_* g_j(\theta) \leq f_j(\theta) \leq d^* g_j(\theta) \text{ a.e.}, \quad g_j(\theta) := |\theta|^{2-jh}.$$

Set

$$\tilde{\mathcal{T}}_n := c_0 T_n(g_0) + c_1 h^h T_n(g_1) + c_2 h^{2h} T_n(g_2) + \dots + c_{n-1} h^{(n-1)h} T_n(g_{n-1}), \quad (2)$$

where the constants c_0, c_1, \dots, c_{n-1} belong to the interval $[c_*, c^*]$, $c^* \geq c_* > 0$, and are independent of n , and $h := \frac{1}{n}$. Then \mathcal{T}_n as in (1) and $\tilde{\mathcal{T}}_n$ are both Hermitian positive definite and in addition

$$d_* \tilde{\mathcal{T}}_n \leq \mathcal{T}_n \leq d^* \tilde{\mathcal{T}}_n.$$

Consequently, we have,

$$\begin{aligned} d_* \lambda_{\min}(\tilde{\mathcal{T}}_n) &\leq \lambda_{\min}(\mathcal{T}_n) \leq d^* \lambda_{\min}(\tilde{\mathcal{T}}_n), \\ d_* \lambda_{\max}(\tilde{\mathcal{T}}_n) &\leq \lambda_{\max}(\mathcal{T}_n) \leq d^* \lambda_{\max}(\tilde{\mathcal{T}}_n), \\ \frac{d_*}{d^*} \cdot \mu_2(\tilde{\mathcal{T}}_n) &\leq \mu_2(\mathcal{T}_n) \leq \frac{d^*}{d_*} \cdot \mu_2(\tilde{\mathcal{T}}_n). \end{aligned}$$

Proof: Taking into account that f_j, g_j are nonnegative a.e. and not identically zero a.e. from the fact that $T_n(\cdot)$ is LPO for any size n in the strong sense, we infer that $T_n(f_j)$ is Hermitian positive definite for $j = 0, \dots, n-1$, and that $T_n(g_j)$ is real symmetric positive definite, owing to the additional fact that g_j is also even for any $j = 0, \dots, n-1$. Consequently, both \mathcal{T}_n and $\tilde{\mathcal{T}}_n$ are positive definite, the first being generically Hermitian and the second being also real symmetric, since they are linear combinations with positive coefficients

of Hermitian positive definite matrices (real symmetric positive definite matrices in the second case).

Now, any linear combination with positive coefficients of LPOs is a new LPO, so that given

$$F_n(\theta) := \sum_{j=0}^{n-1} c_j h^{jh} f_j(\theta), \quad \tilde{F}_n(\theta) := \sum_{j=0}^{n-1} c_j h^{jh} g_j(\theta),$$

$d_* \tilde{F}_n(\theta) \leq F_n(\theta) \leq d^* \tilde{F}_n(\theta)$ a.e. is implied. By the linearity of the operator $T_n(\cdot)$ we easily obtain $\mathcal{T}_n = T_n(F_n)$ and $\tilde{\mathcal{T}}_n = T_n(\tilde{F}_n)$. As a consequence, taking into account the monotonicity, we deduce

$$d_* \tilde{\mathcal{T}}_n \leq \mathcal{T}_n \leq d^* \tilde{\mathcal{T}}_n, \quad (3)$$

while the other four relations are directly implied by the one in (3), with derivation steps as done in Ref. [16], in a slightly different setting. With this, the proof of the theorem is concluded. \blacksquare

The previous reduction theorem allows one to shift the focus of the considered class of problems \mathcal{T}_n , to the simpler class of matrices $\tilde{\mathcal{T}}_n$, with reference to the specific generating function $\tilde{F}_n(\theta)$.

For the very same reason, since the constants c_0, c_1, \dots, c_{n-1} belong to the interval $[c_*, c^*]$, $c^* \geq c_* > 0$, and are independent of n , the asymptotic study can be simplified further and reduced to the analysis of $\hat{\mathcal{T}}_n$ with $\hat{\mathcal{T}}_n := T_n(\hat{F}_n)$, and

$$\hat{F}_n(\theta) := \sum_{j=0}^{n-1} h^{jh} g_j(\theta), \quad (4)$$

in accordance to the following result, whose proof mimics the same steps of the previous one.

Theorem 3.2: For $j = 0, \dots, n-1$, let c_j be positive numbers for which there exist positive constants c^*, c_* independent of n , with

$$0 < c_* \leq c_j \leq c^*.$$

Set

$$\hat{\mathcal{T}}_n := T_n(g_0) + h^h T_n(g_1) + h^{2h} T_n(g_2) + \dots + h^{(n-1)h} T_n(g_{n-1}).$$

Then $\hat{\mathcal{T}}_n$ and $\tilde{\mathcal{T}}_n$ as in (2) are both Hermitian positive definite, in addition

$$c_* \hat{\mathcal{T}}_n \leq \tilde{\mathcal{T}}_n \leq c^* \hat{\mathcal{T}}_n.$$

Consequently, we have

$$\begin{aligned} c_* \lambda_{\min}(\hat{\mathcal{T}}_n) &\leq \lambda_{\min}(\tilde{\mathcal{T}}_n) \leq c^* \lambda_{\min}(\hat{\mathcal{T}}_n), \\ c_* \lambda_{\max}(\hat{\mathcal{T}}_n) &\leq \lambda_{\max}(\tilde{\mathcal{T}}_n) \leq c^* \lambda_{\max}(\hat{\mathcal{T}}_n), \end{aligned}$$

$$\frac{c_*}{c^*} \cdot \mu_2(\hat{\mathcal{T}}_n) \leq \mu_2(\tilde{\mathcal{T}}_n) \leq \frac{c^*}{c_*} \cdot \mu_2(\hat{\mathcal{T}}_n).$$

The rest of the section deals with the more specific case of the asymptotic spectral analysis of $\hat{\mathcal{T}}_n$. The next result shows asymptotic estimates for the extreme eigenvalues of $\hat{\mathcal{T}}_n$. We aim at studying the asymptotic behaviour of the extreme eigenvalues of $\hat{\mathcal{T}}_n = T_n(\hat{F}_n)$ and in particular at proving that $\lambda_{\min}(T_n(\hat{F}_n)) \sim h$, which means that the limsup and the liminf of $\lambda_{\min}(T_n(\hat{F}_n))/h$ are both positive and bounded as $n \rightarrow \infty$. For reaching this goal we consider two preparatory lemmas.

Lemma 3.3: *For all $\alpha_j \in (0, 1]$ and all natural n , there exists a real matrix $R_{n,j}$ such that*

$$T_n(|\theta|^{2-\alpha_j})h^{\alpha_j} \leq T_n(|\theta|^2) + R_{n,j},$$

satisfying the inequality

$$\rho(R_{n,j}) = \|R_{n,j}\|_2 \leq \frac{\alpha_j}{3\pi(3-\alpha_j)} h^2.$$

Proof: We first observe that $|\theta|^{2-\alpha_j}h^{\alpha_j} \leq |\theta|^2$ if and only if $h \leq |\theta|$, therefore

$$|\theta|^{2-\alpha_j}h^{\alpha_j} \leq |\theta|^2 + \psi_{n,j}(\theta)$$

where $\psi_{n,j}(\theta) := \chi_{[-h,h]}(\theta)\{|\theta|^{2-\alpha_j}h^{\alpha_j} - |\theta|^2\}$. Since $T_n: L^1(-\pi, \pi) \rightarrow \mathcal{M}_n(\mathbb{C})$ is a LPO, we deduce that

$$T_n(|\theta|^{2-\alpha_j})h^{\alpha_j} \leq T_n(|\theta|^2) + R_{n,j},$$

where $R_{n,j} := T_n(\psi_{n,j})$, which is a real and symmetric matrix since $\psi_{n,j}$ is a real-valued and even function.

Now we evaluate $\rho(R_{n,j}) = \|R_{n,j}\|_2$, for doing that we bound the k th Fourier coefficient of $\psi_{n,j}$, which we called $\mathfrak{a}_k(\psi_{n,j})$,

$$\begin{aligned} |\mathfrak{a}_k(\psi_{n,j})| &= \left| \frac{1}{2\pi} \int_{-h}^h (|\theta|^{2-\alpha_j}h^{\alpha_j} - |\theta|^2)e^{-ik\theta} d\theta \right| \\ &\leq \frac{1}{2\pi} \int_{-h}^h |\theta|^{2-\alpha_j}(h^{\alpha_j} - |\theta|^{\alpha_j}) d\theta \\ &= \frac{1}{\pi} \int_0^h (\theta^{2-\alpha_j}h^{\alpha_j} - \theta^2) d\theta \\ &= \frac{\alpha_j}{3\pi(3-\alpha_j)} h^3. \end{aligned}$$

Therefore,

$$\rho(R_{n,j}) = \|R_{n,j}\|_2 \leq \|R_{n,j}\|_1 = \max_s \sum_{k=0}^{n-1} |\mathfrak{a}_{s-k}(\psi_{n,j})| \leq \frac{\alpha_j}{3\pi(3-\alpha_j)} h^2,$$

which concludes the proof. ■

Lemma 3.4: For an entire number $q \geq 1$ let $M_{n,q} := \frac{1}{q} \sum_{j=0}^{q-1} T_n(|\theta|^{2-\alpha_j}) h^{\alpha_j}$ with $\alpha_0, \dots, \alpha_{q-1} \in [0, 1]$. Then

$$M_{n,q} \leq T_n(|\theta|^2) + R_n,$$

where $R_n := \sum_{j=0}^{q-1} R_{n,j}$ with $R_{n,j}$ as in Lemma 3.3, and

$$\begin{aligned} \lambda_{\min}(M_{n,q}) &\leq \lambda_{\min}(T_n(|\theta|^2)) + \frac{h^2}{\pi q} \sum_{j=0}^{q-1} \frac{\alpha_j}{\alpha_j + 1} \\ &\sim h^2. \end{aligned}$$

Proof: Let $x_0 \in \mathbb{R}^n$ be an eigenvector of $T_n(|\theta|^2)$ related to $\lambda_0 := \lambda_{\min}(T_n(|\theta|^2))$, that is, $T_n(|\theta|^2)x_0 = \lambda_0 x_0$. Assume also that $\|x_0\|_2 = 1$. From Lemma 3.3, we know that

$$\begin{aligned} M_{n,q} &= \frac{1}{q} \sum_{j=0}^{q-1} T_n(|\theta|^{2-\alpha_j}) h^{\alpha_j} \\ &\leq T_n(|\theta|^2) + \frac{1}{q} \sum_{j=0}^{q-1} R_{n,j} \\ &= T_n(|\theta|^2) + \frac{1}{q} R_n. \end{aligned}$$

Hence we obtain

$$\begin{aligned} \lambda_{\min}(M_{n,q}) &= \min_{\|x\|_2=1} x^* M_{n,q} x \leq x_0^* M_{n,q} x_0 \\ &\leq x_0^* T_n(|\theta|^2) x_0 + \frac{1}{q} x_0^* R_n x_0 \\ &\leq \lambda_0 + \frac{1}{q} \rho(R_n) \\ &= \lambda_0 + \frac{1}{q} \sum_{j=0}^{q-1} \|R_{n,j}\|_2 \\ &\leq \lambda_0 + \frac{\alpha_j}{3\pi(3-\alpha_j)} h^2. \end{aligned}$$

Finally, using that $\lambda_0 \sim h^2$ we finish the proof. ■

Theorem 3.5: Let $M_n := hT_n(\hat{F}_n)$. Then

$$\lambda_{\min}(M_n) \leq \lambda_{\min}(T_n(|\theta|^2)) + \frac{h^3}{\pi} \sum_{j=0}^{n-1} \frac{jh}{jh+1} \sim h^2.$$

Proof: It is sufficient to invoke Lemma 3.4 with $q = n$ and $\alpha_j = jh$. ■

Theorem 3.6: Suppose that $\lambda_1(\hat{\mathcal{T}}_n) \leq \dots \leq \lambda_n(\hat{\mathcal{T}}_n)$. Then, as $n \rightarrow \infty$,

$$\lambda_1(\hat{\mathcal{T}}_n) = O(h) \quad \text{and} \quad \lambda_n(\hat{\mathcal{T}}_n) \leq \frac{\pi(n\pi - 1)}{\log(\pi n)} + O(h \log(n)).$$

Proof: From [5, Th.2.1], we know that

$$\lambda_1(\hat{\mathcal{T}}_n) \leq kh + O(h^2),$$

where k is a positive constant. Hence the assertion $\lambda_1(\hat{\mathcal{T}}_n) = O(h)$ follows.

Note that $e^{-x} \leq 1 - x + \frac{1}{2}x^2$ for $x \in (0, 1)$, hence for every sufficiently large n , we have

$$\begin{aligned} 1 - \left(\frac{1}{n|\theta|}\right)^h &= 1 - \exp(-h \log(n|\theta|)) \\ &\geq h \log(n|\theta|) - \frac{1}{2}h^2 \log^2(n|\theta|). \end{aligned} \quad (5)$$

Using (5), the representation for \hat{F}_n given in Ref. [5, Sc.2], and assuming that $n|\theta| > 1$, we obtain

$$\begin{aligned} \hat{F}_n(\theta) &= \theta^2 \sum_{j=0}^{n-1} |\theta|^{-jh} h^j = \theta^2 \frac{1 - \frac{1}{n|\theta|}}{1 - \left(\frac{1}{n|\theta|}\right)^h} \\ &\leq \frac{\theta^2 \left(1 - \frac{1}{n|\theta|}\right)}{h \log(n|\theta|) \left(1 - \frac{1}{2}h \log(n|\theta|)\right)} \\ &= \frac{n|\theta|(n|\theta| - 1)}{\log(n|\theta|)} \times \frac{h}{1 - \frac{1}{2}h \log(n|\theta|)}. \end{aligned} \quad (6)$$

Consider the function

$$u(x) \equiv \frac{x(x-1)}{\log(x)} \quad (x > 1).$$

From elementary calculus, we know that u is increasing for $x > 1$. Therefore, taking $x = n|\theta|$ and recalling that $|\theta| \in [0, \pi]$, the inequality (6) produces

$$\begin{aligned} \hat{F}_n(\theta) &\leq \frac{\pi(n\pi - 1)}{\log(\pi n)} \times \frac{1}{1 - \frac{1}{2}h \log(\pi n)}, \\ &= \frac{\pi(n\pi - 1)}{\log(\pi n)} + O(h \log(n)). \end{aligned} \quad (7)$$

Finally, assume that $n|\theta| < 1$. A similar calculation shows that

$$\hat{F}_n(\theta) \leq 2h\pi. \quad (8)$$

Combining (7), (8) with $\lambda_n(\hat{\mathcal{T}}_n) = \|\hat{\mathcal{T}}_n\|_2 \leq \sup\{|\hat{F}_n(\theta)| : \theta \in [-\pi, \pi]\}$ the proof is concluded. ■

4. Numerical experiments

In this section, we numerically check the theoretical findings provided in Section 3. With this aim, we first calculate the entries of the matrices $T_n(\hat{F}_n)$ and $T_n(\eta)$ for $\eta(\theta) := \theta^2$. From (4), the k th Fourier coefficient of the function $\hat{F}_n(\theta)$, named $\alpha_k(\hat{F}_n)$, can be obtained as

$$\alpha_k(\hat{F}_n) = \sum_{j=0}^{n-1} h^{jh} \alpha_k(g_j),$$

where $\alpha_k(g_j)$ is the k th Fourier coefficient of the function $g_j(\theta) = |\theta|^{2-jh}$. Additionally, $\alpha_k(g_j)$ can be exactly calculated with

$$\begin{aligned} \alpha_k(g_j) &= \frac{1}{\pi} \int_0^\pi \theta^{2-jh} \cos(k\theta) \, d\theta \\ &= \frac{\pi^{2-jh}}{3-jh} {}_1H_2 \left(\frac{1}{2}(3-jh); \frac{1}{2}, \frac{1}{2}(5-jh); -\frac{k^2\pi^2}{4} \right) \end{aligned}$$

where ${}_pH_q$ is the well-known Generalized Hypergeometric function that can be found as an internal function, e.g. in the *Mathematica* software. Thus we can exactly calculate the entries of the Toeplitz matrix $T_n(\hat{F}_n)$.

On the other hand, the Fourier coefficients of η can be exactly calculated by

$$\alpha_k(\eta) = \begin{cases} \frac{2}{k^2} \cos(\pi k) + \frac{k^2\pi^2 - 2}{k^3\pi} \sin(\pi k), & k \neq 0; \\ \frac{\pi^2}{3}, & k = 0. \end{cases}$$

Table 1 shows the extreme eigenvalues of $T_n(\hat{F}_n)$ for different values of n . It agrees with the results of Theorem 3.6 and, in particular, shows that $\mu_2(T_n(\hat{F}_n)) = O\left(\frac{(\pi n)^2}{\log(\pi n)}\right)$.

Having in mind that matrices in the form of $T_n(\hat{F}_n)$ arise within distributed-order fractional problems which are typically ill-conditioned, we conclude this section by providing a short discussion on the conditioning of $T_n^{-1}(\eta)T_n(\hat{F}_n)$, i.e. we check how the spectrum changes when preconditioning with a Laplacian-like matrix. Table 2 shows the extreme

Table 1. The extreme eigenvalues and the conditioning of $T_n(\hat{F}_n)$ for different values of n .

n	64	128	256	512	1024	2048
λ_{\min}	$7.8737 \cdot 10^{-2}$	$3.9480 \cdot 10^{-2}$	$1.9768 \cdot 10^{-2}$	$9.8914 \cdot 10^{-3}$	$4.9476 \cdot 10^{-3}$	$2.4743 \cdot 10^{-3}$
λ_{\min}^*	5.0392	5.0534	5.0607	5.0644	5.0663	5.0673
λ_{\max}	120.9373	212.8457	380.1275	687.1094	1 254.2460	2 307.9670
λ_{\max}^*	1.015	1.010	1.006	1.004	1.002	1.001
μ_2	1 535.9667	5 391.2724	19 229.1665	69 465.1987	253 507.4186	932 790.7960
μ_2^*	0.2015	0.1999	0.1989	0.1982	0.1978	0.1976

Note: Here we used the notation $\lambda_{\min}^* = n\lambda_{\min}$, $\lambda_{\max}^* = \frac{\log(\pi n)}{\pi^2 n} \lambda_{\max}$, and $\mu_2^* = \frac{\log(\pi n)}{(\pi n)^2} \mu_2$.

Table 2. The extreme eigenvalues and the conditioning of $T_n^{-1}(\eta)T_n(\hat{F}_n)$ where $\eta(\theta) = \theta^2$, for different values of n .

n	64	128	256	512	1024	2048
λ_{\min}	15.4546	26.5447	46.4058	82.3378	147.9148	268.6040
λ_{\min}^\dagger	1.004	1.006	1.005	1.003	1.001	1.000
λ_{\max}	1 793.0355	6 479.2722	23 557.6771	86 165.4914	316 954.9557	1 175 952.6713
λ_{\max}^\dagger	2.3217	2.3715	2.4048	2.4268	2.4412	2.4587
μ_2	116.0198	244.0896	507.6456	1 046.4872	2 142.8207	4 378.0162
μ_2^\dagger	1.8128	1.9069	1.9830	2.0439	2.0926	2.1377

Note: Here we used the notation $\lambda_{\min}^\dagger = h \log n \lambda_{\min}$, $\lambda_{\max}^\dagger = h^2 \log(\pi n) \lambda_{\max}$, and $\mu_2^\dagger = h \mu_2$.

eigenvalues of $T_n^{-1}(\eta)T_n(\hat{F}_n)$ for different values of n . It suggests that

$$\lambda_{\min}(T_n^{-1}(\eta)T_n(\hat{F}_n)) = O\left(\frac{n}{\log n}\right) \quad \text{and} \quad \lambda_{\max}(T_n^{-1}(\eta)T_n(\hat{F}_n)) = O\left(\frac{n^2}{\log(\pi n)}\right).$$

From this results, we expect that $\mu_2(T_n^{-1}(\eta)T_n(\hat{F}_n)) = O(n)$ which means that η is not acting as an effective preconditioning function.

Figure 1 shows the eigenvalues of $T_n(\hat{F}_n)$ and $T_n^{-1}(\eta)T_n(\hat{F}_n)$ for $n = 1024$, and from them, it is immediately clear that the largest eigenvalue of $T_n(\hat{F}_n)$ is magnified after preconditioning and that the preconditioned spectrum is far from being well-clustered.

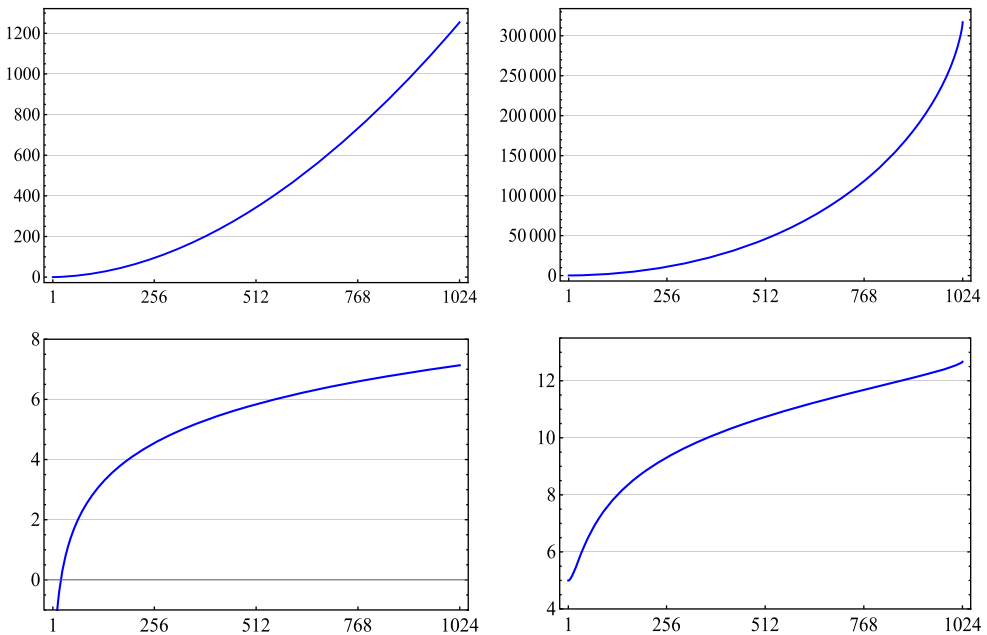


Figure 1. The eigenvalues of $T_n(\hat{F}_n)$ and of $T_n^{-1}(\eta)T_n(\hat{F}_n)$ where $\eta(\theta) = \theta^2$, for $n = 1024$. Regular scale (top) and logarithmic scale (bottom).

5. Conclusions

In this work, we have considered a novel type of spectral problem involving Toeplitz structures and arising in the numerical approximation of distributed-order fractional differential equations. The spectral study of the matrices under consideration has been reduced to the study of the matrix

$$T_n(g_0) + h^h T_n(g_1) + h^{2h} T_n(g_2) + \dots + h^{(n-1)h} T_n(g_{n-1}),$$

where $h = \frac{1}{n}$, $g_j(\theta) = |\theta|^{2-jh}$, and $j = 0, \dots, n-1$. Because the resulting generating function depends on n , the standard theory cannot be applied, and the analysis has been performed using new ideas. Few selected numerical experiments have been presented and critically discussed. Many open questions remain: we can consider, for instance, the use of the given spectral information in a context of Krylov preconditioning or multigrid design, for large linear systems coming from FDEs with distributed order, and the extension of the proposed analysis in a multidimensional context, when the spatial derivatives belong to a d -dimensional domain with $d \geq 2$. These lines of research will be the subject of future investigations.

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ORCID

Manuel Bogoya  <http://orcid.org/0000-0003-3551-8152>

Sergei Grudsky  <http://orcid.org/0000-0002-3748-5449>

Mariarosa Mazza  <http://orcid.org/0000-0002-8505-6788>

Stefano Serra-Capizzano  <http://orcid.org/0000-0001-9477-109X>

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