Are the Eigenvalues of Banded Symmetric Toeplitz Matrices Known in Almost Closed Form?

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ABSTRACT

Bogoya, Böttcher, Grudsky, and Maximenko have recently obtained for the eigenvalues of a Toeplitz matrix, under suitable assumptions on the generating function, the precise asymptotic expansion as the matrix size goes to infinity. In this article we provide numerical evidence that some of these assumptions can be relaxed. Moreover, based on the eigenvalue asymptotics, we devise an extrapolation algorithm for computing the eigenvalues of banded symmetric Toeplitz matrices with a high level of accuracy and a relatively low computational cost.

KEYWORDS

eigenvalue asymptotics; eigenvalues; extrapolation; polynomial interpolation; Toeplitz matrix

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1. Introduction

A matrix of the form

$$[a_{i-j}]_{i,j=1}^{n} = \begin{bmatrix} a_0 & a_{-1} & a_{-2} & \cdots & a_{-(n-1)} \\ a_1 & \ddots & \ddots & \ddots & \vdots \\ a_2 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & a_{-2} \\ \vdots & & \ddots & \ddots & \ddots & a_{-1} \\ a_{n-1} & \cdots & \cdots & a_2 & a_1 & a_0 \end{bmatrix},$$

whose entries are constant along each diagonal, is called a Toeplitz matrix. Given a function $f: [-\pi, \pi] \to \mathbb{C}$ belonging to $L^1([-\pi, \pi])$, the *n*th Toeplitz matrix associated with f is defined as

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

where the numbers \hat{f}_k are the Fourier coefficients of f,

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

We refer to $\{T_n(f)\}_n$ as the Toeplitz sequence generated by f, which in turn is called the generating function or the symbol of $\{T_n(f)\}_n$. In the case where f is real, all the matrices $T_n(f)$ are Hermitian and much is known about their spectral properties, from the localization of the eigenvalues to the asymptotic spectral distribution in the Weyl sense; see [Böttcher and Silbermann 99, Garoni and Serra-Capizzano 17] and the references therein. The present article focuses on the case where f is a real cosine trigonometric polynomial (RCTP), that is, a function of the form

$$f(\theta) = \hat{f}_0 + 2\sum_{k=1}^m \hat{f}_k \cos(k\theta), \qquad \hat{f}_0, \, \hat{f}_1, \dots, \, \hat{f}_m \in \mathbb{R},$$
$$m \in \mathbb{N}$$

We say that the RCTP f is monotone if it is either increasing or decreasing over the interval $[0, \pi]$. The *n*th Toeplitz matrix generated by f is the real symmetric banded matrix given by

In [Bogoya et al. 15a, Bogoya et al. 17, Böttcher et al. 10] it was proved that if the RCTP f is monotone and

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satisfies certain additional assumptions, which include the requirements that $f'(\theta) \neq 0$ for $\theta \in (0, \pi)$ and $f''(\theta) \neq 0$ for $\theta \in \{0, \pi\}$, then, for every integer $\alpha \ge 0$, every *n* and every j = 1, ..., n, the following asymptotic expansion holds:

$$\lambda_{j}(T_{n}(f)) = f(\theta_{j,n}) + \sum_{k=1}^{\alpha} c_{k}(\theta_{j,n})h^{k} + E_{j,n,\alpha}, \quad (1-1)$$

where:

- The eigenvalues of $T_n(f)$ are arranged in nondecreasing or non-increasing order, depending on whether *f* is increasing or decreasing.
- $\{c_k\}_{k=1,2,\dots}$ is a sequence of functions from $[0, \pi]$ to \mathbb{R} which depends only on *f*.
- $h = \frac{1}{n+1}$ and $\theta_{j,n} = \frac{j\pi}{n+1} = j\pi h$. $E_{j,n,\alpha} = O(h^{\alpha+1})$ is the remainder (the error), which satisfies the inequality $|E_{j,n,\alpha}| \leq C_{\alpha}h^{\alpha+1}$ for some constant C_{α} depending only on α and f.

The symbols

$$f_q(\theta) = (2 - 2\cos\theta)^q, \qquad q = 1, 2, \dots$$
 (1-2)

arise in the discretization of differential equations and are therefore of particular interest. Unfortunately, for these symbols the requirement that $f''(0) \neq 0$ is not satisfied if $q \ge 2$. The first purpose of this article is to provide numerical evidence that the higher-order approximation (1-1)holds even in this "degenerate case." Actually, based on our numerical experiments, we conjecture that (1-1) holds for all monotone RCTPs f.

In [Bogoya et al. 15a], the authors also briefly mentioned that the asymptotic expansion (1-1) can be used to compute an accurate approximation of $\lambda_i(T_n(f))$ for very large *n*, provided the values $\lambda_{j_1}(T_{n_1}(f)), \lambda_{j_2}(T_{n_2}(f))$, $\lambda_{j_3}(T_{n_3}(f))$ are available for moderately sized n_1, n_2, n_3 with $\theta_{j_1,n_1} = \theta_{j_2,n_2} = \theta_{j_3,n_3} = \theta_{j,n}$. The second and main purpose of this article is to carry out this idea and to support it by numerical experiments accompanied by an appropriate error analysis. In particular, we devise an algorithm to compute $\lambda_i(T_n(f))$ with a high level of accuracy and a relatively low computational cost. The algorithm is completely analogous to the extrapolation procedure which is employed in the context of Romberg integration to obtain high precision approximations of an integral from a few coarse trapezoidal approximations [Stoer and Bulirsch 02, Section 3.4]. In this regard, the asymptotic expansion (1-1) plays here the same role as the Euler-Maclaurin summation formula [Stoer and Bulirsch 02, Section 3.3].

In the case where the monotonicity assumption on fis violated, a first-order asymptotic formula for the eigenvalues was established by Bogoya, Böttcher, Grudsky, and

Maximenko in [Bogoya et al. 15b]. In particular, following the argument used for the proof of [Bogoya et al. 15b, Theorem 1.6], one can show that for every RCTP f, every *n* and every $j = 1, \ldots, n$, we have

$$\lambda_{\rho_n(j)}(T_n(f)) = f(\theta_{j,n}) + E_{j,n,0},$$
(1-3)

where:

- The eigenvalues of $T_n(f)$ are arranged in nondecreasing order, $\lambda_1(T_n(f)) \leq \cdots \leq \lambda_n(T_n(f))$.
- $\rho_n = \sigma_n^{-1}$, where σ_n is a permutation of $\{1, \ldots, n\}$ such that $f(\theta_{\sigma_n(1),n}) \leq \cdots \leq f(\theta_{\sigma_n(n),n})$.
- $h = \frac{1}{n+1}$ and $\theta_{j,n} = \frac{j\pi}{n+1} = j\pi h$.
- $E_{j,n,0} = O(h)$ is the error, which satisfies the inequality $|E_{i,n,0}| \leq C_0 h$ for some constant C_0 depending only on *f*.

The third and last purpose of this article is to formulate, on the basis of numerical experiments, a conjecture on the higher-order asymptotics of the eigenvalues if the monotonicity assumption on f is not in force. We also illustrate how this conjecture can be used along with our extrapolation algorithm in order to compute some of the eigenvalues of $T_n(f)$ in the case where f is non-monotone.

1.1. Ideas from numerical linear algebra

Before entering into the details of the article, we allow us a digression. Our aim is to highlight that the first-order expansion (1-3) may be proved by purely linear algebra arguments in combination with the results about the socalled quantile function obtained in [Bogoya et al. 15b, Bogoya et al. 16]. Let us outline the scheme of a linear algebra proof of this kind. We will make use of the so-called τ matrices and the related properties [Bini and Capovani 83, Serra-Capizzano 96].

Let $\tau_n(f)$ be the τ matrix of size *n* generated by *f*. Then, $\tau_n(f)$ is a real symmetric matrix with the following properties:

• $T_n(f) = \tau_n(f) + R_n^+ + R_n^-$, where R_n^+ is a symmetric nonnegative definite matrix of rank k^+ , R_n^- is a symmetric nonpositive definite matrix of rank k^- , and $k^+ + k^- \leq 2(m-1)$, with *m* being the degree of f.

• The eigenvalues of $\tau_n(f)$ are $f(\theta_{j,n})$, j = 1, ..., n. Using a classical interlacing theorem for the eigenvalues (see [Bhatia 97, Exercise III.2.4] or [Garoni and Serra-Capizzano 17, Theorem 2.12]), we obtain

$$f(\theta_{\sigma_n(j-k^-),n}) \le \lambda_j(T_n(f)) \le f(\theta_{\sigma_n(j+k^+),n}),$$

$$j = k^- + 1, \dots, n - k^+.$$
(1-4)

Moreover, it is known that

$$\lambda_j(T_n(f)) \in [m_f, M_f], \quad j = 1, ..., n, \quad (1-5)$$





Figure 1. Example 1: Errors $E_{j,n,0}$ and scaled errors $E_{j,n,0}/h$ versus $\theta_{j,n}$ for j = 1, ..., n and n = 100, 200, 400 in the case of the symbol $f(\theta) = (2 - 2\cos\theta)^2$.

where $m_f = \min f$ and $M_f = \max f$; see [Böttcher and Silbermann 99, Garoni and Serra-Capizzano 17]. Considering that f is an RCTP and hence a Lipschitz continuous function, the result (1–3) intuitively follows from (1–4) and (1–5). For a formal derivation, however, it is necessary to resort to the quantile function of f, which is monotone and Lipschitz continuous whenever f is Lipschitz continuous; see [Bogoya et al. 15b, Proposition 2.7].

The relation (1-4) is known in the numerical linear algebra community since more than 30 years and was used in [Serra-Capizzano 96] to study the asymptotics of the extreme eigenvalues of Toeplitz matrices. In particular, if $\alpha \ge 2$ denotes the minimum order of the zeros of $f - \min f$, it was proved in [Serra-Capizzano 96] that the errors $E_{j,n,0}$ corresponding to the smallest eigenvalues of $T_n(f)$ are $O(h^{\alpha})$ and not only O(h). More precisely, whenever j is constant with respect to n, we have $|E_{j,n,0}| \le c_j h^{\alpha}$ for some constant c_j depending only on f and j.

2. Numerical experiments in support of the asymptotic expansion

We present in this section a few numerical examples, with the purpose of supporting the conjecture that the asymptotic expansion (1–1) is satisfied for all monotone RCTPs f, including those which do not meet the requirements $f'(\theta) \neq 0$ for $\theta \in (0, \pi)$ and $f''(\theta) \neq 0$ for $\theta \in \{0, \pi\}$.

Example 1. Let f be the monotone RCTP defined by (1-2) for q = 2,





Note that f''(0) = 0. The expansion (1–1) with $\alpha = 1$ would say that, for every *n* and every j = 1, ..., n,

$$\lambda_j(T_n(f)) - f(\theta_{j,n}) = E_{j,n,0}$$

= $c_1(\theta_{j,n})h + E_{j,n,1}$, (2-6)

where $|E_{j,n,1}| \leq C_1 h^2$ and both the function $c_1 : [0, \pi] \rightarrow \mathbb{R}$ and the constant C_1 depend only on f. In particular, the scaled errors $E_{j,n,0}/h$ should be equal to the equispaced samples $c_1(\theta_{j,n})$ (and should therefore reproduce the graph of the function c_1) in the limit where $n \rightarrow \infty$. In Figure 1 we plot the errors $E_{j,n,0}$ and the scaled errors $E_{j,n,0}/h$ versus $\theta_{j,n}$ for $j = 1, \ldots, n$ and n = 100, 200, 400. It is clear that the scaled errors overlap perfectly, thus supporting the conjecture that the expansion (2–6) holds despite the fact that f''(0) = 0. In particular, the right pane of Figure 1 displays the graph of c_1 over $[0, \pi]$.

Example 2. Let

$$f(\theta) = 1 + 24\cos\theta - 12\cos(2\theta) + 8\cos(3\theta)$$
$$-3\cos(4\theta).$$

The function f is a monotone decreasing RCTP such that $f'(\pi/2) = f''(\pi/2) = f''(0) = 0$. Figure 2 is obtained in the same way as Figure 1. Again, we see that the scaled errors overlap perfectly, thus supporting the conjecture that the expansion (2–6) holds even for this function f, despite the fact that f violates both the conditions $f'(\theta) \neq 0$ for $\theta \in (0, \pi)$ and $f''(\theta) \neq 0$ for $\theta \in \{0, \pi\}$.

Example 3. Let *f* be the same as in Example 2. The expansion (1-1) with $\alpha = 2$ would say that, for every *n* and



Figure 2. Example 2: Errors $E_{j,n,0}$ and scaled errors $E_{j,n,0}/h$ versus $\theta_{j,n}$ for j = 1, ..., n and n = 100, 200, 400 in the case of the symbol $f(\theta) = 1 + 24 \cos \theta - 12 \cos(2\theta) + 8 \cos(3\theta) - 3 \cos(4\theta)$.

every
$$j = 1, ..., n$$
,
 $\lambda_j(T_n(f)) - f(\theta_{j,n}) - c_1(\theta_{j,n})h = E_{j,n,1}$
 $= c_2(\theta_{j,n})h^2 + E_{j,n,2},$
(2-7)

where $|E_{j,n,2}| \leq C_2 h^3$ and both the function $c_2 : [0, \pi] \rightarrow \mathbb{R}$ and the constant C_2 depend only on f. In particular, the scaled errors $E_{j,n,1}/h^2$ should be equal to the equispaced samples $c_2(\theta_{j,n})$ (and should therefore reproduce the graph of the function c_2) in the limit where $n \rightarrow \infty$. Unfortunately, the values $E_{j,n,1}$ are not available, because the function c_1 is unknown. To work around this problem, we fix $n' \gg n$ such that (n' + 1) is a multiple of (n + 1) and we approximate $E_{j,n,1}$ by

$$\tilde{E}_{j,n,1} = \lambda_j(T_n(f)) - f(\theta_{j,n}) - \tilde{c}_1(\theta_{j,n})h,$$

where \tilde{c}_1 is the approximation of c_1 obtained from the scaled errors $E_{j',n',0}/h'$ corresponding to the fine parameter n'. In other words, \tilde{c}_1 is defined at every point $\theta_{j',n'}$ as

$$\tilde{c}_{1}(\theta_{j',n'}) = \frac{E_{j',n',0}}{h'} = \frac{\lambda_{j'}(T_{n'}(f)) - f(\theta_{j',n'})}{h'}$$
$$= c_{1}(\theta_{j',n'}) + \frac{E_{j',n',1}}{h'}, \quad j' = 1, \dots, n', \quad h' = \frac{1}{n'+1}.$$

Note that \tilde{c}_1 is also defined at every point $\theta_{j,n}$, because (n' + 1) is a multiple of (n + 1) and hence every $\theta_{j,n}$ is equal to some $\theta_{j',n'}$ (indeed, $\theta_{j,n} = \theta_{j',n'}$ for $j' = j\frac{n'+1}{n+1}$). When approximating $c_2(\theta_{j,n})$ by $\tilde{E}_{j,n,1}/h^2$ instead of $E_{j,n,1}/h^2$, the error can be estimated as follows:

$$\begin{aligned} \frac{\tilde{E}_{j,n,1}}{h^2} &- c_2(\theta_{j,n}) \\ &= \left| \frac{E_{j,n,1} + h [\tilde{c}_1(\theta_{j,n}) - c_1(\theta_{j,n})]}{h^2} - c_2(\theta_{j,n}) \right| \\ &\leq \left| \frac{E_{j,n,1}}{h^2} - c_2(\theta_{j,n}) \right| + \frac{1}{h} |\tilde{c}_1(\theta_{j,n}) - c_1(\theta_{j,n})| \\ &= \left| \frac{E_{j,n,2}}{h^2} \right| + \frac{1}{h} |\tilde{c}_1(\theta_{j',n'}) - c_1(\theta_{j',n'})| \end{aligned}$$

(here
$$j' = j \frac{n+1}{n+1}$$
 so that $\theta_{j',n'} = \theta_{j,n}$)



$$= \left| \frac{E_{j,n,2}}{h^2} \right| + \frac{1}{h} \left| \frac{E_{j',n',1}}{h'} \right|$$
$$\leq C_2 h + C_1 \frac{h'}{h}.$$

We may then expect that the errors $|\tilde{E}_{j,n,1}/h^2 - c_2(\theta_{j,n})|$ are of the same order as the errors $|E_{j,n,1}/h^2 - c_2(\theta_{j,n})| = |E_{j,n,2}/h^2|$ provided that $h' = O(h^2)$. In Figure 3 we plot the approximated errors $\tilde{E}_{j,n,1}$ and the approximated scaled errors $\tilde{E}_{j,n,1}/h^2$ versus $\theta_{j,n}$ for j = 1, ..., n and n = 100, 200, 400, with $n' = \lceil \frac{n+1}{12} \rceil (n+1) - 1$. With this choice of n', we ensure that (n'+1) is a multiple of (n+1) and $h' \approx 12h^2$ for all n. The figure reveals that the approximated scaled errors converge to a limit function c_2 , thus supporting the conjecture that the expansion (2-7) holds despite the fact that f violates both the conditions $f'(\theta) \neq 0$ for $\theta \in (0, \pi)$ and $f''(\theta) \neq 0$ for $\theta \in \{0, \pi\}$.

Algorithm for computing the eigenvalues with high accuracy

In Section 2 we showed through numerical examples that the asymptotic expansion (1-1) is likely to be satisfied for every monotone RCTP f. We now illustrate how (1-1) can be used to compute an accurate approximation of $\lambda_j(T_n(f))$ for large n.

Let *f* be a monotone RCTP, fix $n \in \mathbb{N}$ and $j \in \{1, ..., n\}$. Suppose $\lambda_{j_1}(T_{n_1}(f)), ..., \lambda_{j_m}(T_{n_m}(f))$ are available for some $(j_1, n_1), ..., (j_m, n_m)$ such that $j_1h_1 = \cdots = j_mh_m = jh$, where $h_1 = \frac{1}{n_1+1}, ..., h_m = \frac{1}{n_m+1}, h = \frac{1}{n+1}$. In this situation we have $\theta_{j_1,n_1} = \cdots = \theta_{j_m,n_m} = \theta_{j,n} = \bar{\theta}$ for some $\bar{\theta} \in (0, \pi)$, and the application of (1-1) with $\alpha = m$ yields

$$E_{j_{i},n_{i},0} = \lambda_{j_{i}}(T_{n_{i}}(f)) - f(\bar{\theta})$$

$$= \sum_{k=1}^{m} c_{k}(\bar{\theta})h_{i}^{k} + E_{j_{i},n_{i},m}, \quad i = 1, \dots, m, (3-8)$$

$$E_{j,n,0} = \lambda_{j}(T_{n}(f)) - f(\bar{\theta})$$

$$= \sum_{k=1}^{m} c_{k}(\bar{\theta})h^{k} + E_{j,n,m}, \quad (3-9)$$



Figure 3. Example 3: Approximated errors $\tilde{E}_{j,n,1}$ and approximated scaled errors $\tilde{E}_{j,n,1}/h^2$ versus $\theta_{j,n}$ for j = 1, ..., n and n = 100, 200, 400 in the case of the symbol $f(\theta) = 1 + 24 \cos \theta - 12 \cos(2\theta) + 8 \cos(3\theta) - 3 \cos(4\theta)$.

where

$$E_{j_i,n_i,m}| \le C_m h_i^{m+1}, \qquad i = 1, \dots, m, \quad (3-10)$$

 $|E_{j,n,m}| \le C_m h^{m+1}. \quad (3-11)$

We are interested in a linear combination of the errors $E_{j_i,n_i,0}$ which "reconstructs" as much as possible the error $E_{j,n,0}$. More precisely, we look for a linear combination

$$\sum_{i=1}^{m} a_i E_{j_i, n_i, 0} = \sum_{k=1}^{m} c_k(\bar{\theta}) \sum_{i=1}^{m} a_i h_i^k + \sum_{i=1}^{m} a_i E_{j_i, n_i, m}$$
(3-12)

such that

$$\sum_{i=1}^{m} a_i h_i^k = h^k, \qquad k = 1, \dots, m.$$
(3-13)

If $[\hat{a}_1, \ldots, \hat{a}_m]$ is a vector satisfying the conditions (3–13), then

$$\sum_{i=1}^{m} \hat{a}_i E_{j_i, n_i, 0} = E_{j, n, 0} + \sum_{i=1}^{m} \hat{a}_i E_{j_i, n_i, m} - E_{j, n, m}, \quad (3-14)$$

and in view of (3–10) and (3–11) the linear combination $\sum_{i=1}^{m} \hat{a}_i E_{j_i,n_i,0}$ is supposed to be an accurate reconstruction of $E_{j,n,0}$. This immediately yields the following high precision approximation for $\lambda_j(T_n(f))$:

$$\lambda_{j}(T_{n}(f)) = f(\bar{\theta}) + E_{j,n,0} \approx f(\bar{\theta}) + \sum_{i=1}^{m} \hat{a}_{i} E_{j_{i},n_{i},0}.$$
(3-15)

By (3-10), (3-11), and (3-14), an estimate for the error of this approximation is given by

$$\begin{vmatrix} \lambda_{j}(T_{n}(f)) - f(\bar{\theta}) - \sum_{i=1}^{m} \hat{a}_{i}E_{j_{i},n_{i},0} \end{vmatrix} \\ = \left| E_{j,n,0} - \sum_{i=1}^{m} \hat{a}_{i}E_{j_{i},n_{i},0} \right| = \left| \sum_{i=1}^{m} \hat{a}_{i}E_{j_{i},n_{i},m} - E_{j,n,m} \right| \\ \leq C_{m} \left[\sum_{i=1}^{m} |\hat{a}_{i}|h_{i}^{m+1} + h^{m+1} \right].$$
(3-16)

Theorem 1. There exists a unique vector $[\hat{a}_1, \ldots, \hat{a}_m] \in \mathbb{R}^m$ satisfying the conditions (3–13) and, moreover, the special linear combination $\sum_{i=1}^m \hat{a}_i E_{j_i,n_i,0}$ coincides with hp(h), where p(x) is the interpolation polynomial for the data $(h_1, E_{j_1,n_1,0}/h_1), \ldots, (h_m, E_{j_m,n_m,0}/h_m)$.

Proof. Let $V(h_1, \ldots, h_m)$ be the Vandermonde matrix corresponding to the nodes h_1, \ldots, h_m :

$$V(h_1, \dots, h_m) = \begin{bmatrix} 1 & h_1 & \cdots & h_1^{m-1} \\ 1 & h_2 & \cdots & h_2^{m-1} \\ \vdots & \vdots & & \vdots \\ 1 & h_m & \cdots & h_m^{m-1} \end{bmatrix}.$$

We recall two properties of $V(h_1, \ldots, h_m)$ that can be found, e.g., in [Bevilacqua et al. 92, Chapter 5] or [Davis 75, Chapter II]. First, since it is implicitly assumed that n_1, \ldots, n_m (and hence also h_1, \ldots, h_m) are all distinct, the matrix $V(h_1, \ldots, h_m)$ is invertible. Second, for any $\mathbf{y} = [y_1, \ldots, y_m]^T \in \mathbb{R}^m$, the vector $\mathbf{q} =$ $[V(h_1, \ldots, h_m)]^{-1}\mathbf{y} = [q_1, \ldots, q_m]^T$ is such that q(x) = $q_1 + q_2x + \cdots + q_mx^{m-1}$ is the interpolation polynomial for the data $(h_1, y_1), \ldots, (h_m, y_m)$.

The conditions (3-13) can be rewritten as

$$\begin{bmatrix} h_1 & h_2 & \cdots & h_m \\ h_1^2 & h_2^2 & \cdots & h_m^2 \\ \vdots & \vdots & & \vdots \\ h_1^m & h_2^m & \cdots & h_m^m \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{bmatrix} = \begin{bmatrix} h \\ h^2 \\ \vdots \\ h^m \end{bmatrix}. \quad (3-17)$$

If we define

$$D = \begin{bmatrix} h_1 & & & \\ & h_2 & & \\ & & \ddots & \\ & & & h_m \end{bmatrix},$$

then the matrix A of the linear system (3-17) satisfies

$$A = AD^{-1}D = [V(h_1, \ldots, h_m)]^T D.$$

It follows that *A* is invertible and so the linear system (3-17) has a unique solution $[\hat{a}_1, \ldots, \hat{a}_m]^T$. Moreover, we have

$$A\begin{bmatrix} \hat{a}_1\\ \hat{a}_2\\ \vdots\\ \hat{a}_m \end{bmatrix} = \begin{bmatrix} h\\ h^2\\ \vdots\\ h^m \end{bmatrix}$$
$$\iff [\hat{a}_1, \hat{a}_2, \dots, \hat{a}_m]A^T = [h, h^2, \dots, h^m]$$
$$\iff [\hat{a}_1, \hat{a}_2, \dots, \hat{a}_m] = h[1, h, \dots, h^{m-1}]A^{-T}.$$

If we denote by $p(x) = p_1 + p_2 x + \dots + p_m x^{m-1}$ the interpolation polynomial for the data $(h_1, E_{j_1,n_1,0}/h_1)$, \dots , $(h_m, E_{j_m,n_m,0}/h_m)$, then

$$\sum_{i=1}^{m} \hat{a}_{i} E_{j_{i},n_{i},0}$$

$$= [\hat{a}_{1}, \hat{a}_{2}, \dots, \hat{a}_{m}] \begin{bmatrix} E_{j_{1},n_{1},0} \\ E_{j_{2},n_{2},0} \\ \vdots \\ E_{j_{m},n_{m},0} \end{bmatrix}$$

$$= h[1, h, \dots, h^{m-1}] A^{-T} \begin{bmatrix} E_{j_{1},n_{1},0} \\ E_{j_{2},n_{2},0} \\ \vdots \\ E_{j_{m},n_{m},0} \end{bmatrix}$$

$$= h[1, h, \dots, h^{m-1}][V(h_1, \dots, h_m)]^{-1}D^{-1}\begin{bmatrix} E_{j_1, n_1, 0} \\ E_{j_2, n_2, 0} \\ \vdots \\ E_{j_m, n_m, 0} \end{bmatrix}$$
$$= h[1, h, \dots, h^{m-1}][V(h_1, \dots, h_m)]^{-1}\begin{bmatrix} E_{j_1, n_1, 0}/h_1 \\ E_{j_2, n_2, 0}/h_2 \\ \vdots \\ E_{j_m, n_m, 0}/h_m \end{bmatrix}$$
$$= h[1, h, \dots, h^{m-1}]\begin{bmatrix} p_1 \\ p_2 \\ \vdots \\ p_m \end{bmatrix} = h\sum_{i=1}^m p_i h^{i-1} = hp(h).$$

We remark that *n* is normally much larger than n_1, \ldots, n_m . Indeed, the idea behind the algorithm we are describing here is to obtain a high precision approximation of $\lambda_j(T_n(f))$ at the sole price of computing a few eigenvalues $\lambda_{j_1}(T_{n_1}(f)), \ldots, \lambda_{j_m}(T_{n_m}(f))$ with $n_1, \ldots, n_m \ll n$. Due to the moderate sizes n_1, \ldots, n_m , the latter eigenvalues can be efficiently computed by a standard eigensolver, and the desired approximation of $\lambda_j(T_n(f))$ is then obtained via equation (3–15) with the \hat{a}_i given by Theorem 1, i.e.,

$$\lambda_{j}(T_{n}(f)) = f(\bar{\theta}) + E_{j,n,0} \approx f(\bar{\theta}) + \sum_{i=1}^{m} \hat{a}_{i}E_{j_{i},n_{i},0}$$

= $f(\bar{\theta}) + hp(h).$ (3-18)

An estimate for the error of this approximation is given by (3-16):

$$\begin{aligned} \left| \lambda_{j}(T_{n}(f)) - f(\bar{\theta}) - hp(h) \right| \\ \leq C_{m} \left[\sum_{i=1}^{m} |\hat{a}_{i}| h_{i}^{m+1} + h^{m+1} \right]. \quad (3-19) \end{aligned}$$

The procedure of evaluating the interpolation polynomial p(x) at x = h is referred to as extrapolation, because p(x) is evaluated at a point which lies outside the convex hull of the interpolation nodes h_1, \ldots, h_m . A completely analogous extrapolation procedure is employed in the context of Romberg integration to obtain high precision approximations of an integral from a few coarse trapezoidal approximations; see [Stoer and Bulirsch 02, Section 3.4]. For more details on extrapolation methods, we refer the reader to [Brezinski and Redivo Zaglia 91].

Algorithm 1. With the notation of this article, given f and m + 1 pairs $(j_1, n_1), \ldots, (j_m, n_m), (j, n)$ such that $j_1h_1 = \cdots = j_mh_m = jh$, we compute a high precision approximation of $\lambda_j(T_n(f))$ as follows:

• Compute the eigenvalues $\lambda_{j_1}(T_{n_1}(f)), \dots, \lambda_{j_m}(T_{n_m}(f))$ using a standard eigensolver.

- Compute the errors $E_{\underline{j}_i,n_i,0} = \lambda_{j_i}(T_{n_i}(f)) f(\overline{\theta})$ for $i = 1, \dots, m$, where $\overline{\theta} = \theta_{j,n} = j\pi h$.
- Compute p(h), where p(x) is the interpolation polynomial for the data $(h_i, E_{j_i, n_i, 0}/h_i), i = 1, ..., m$.
- Return $f(\bar{\theta}) + hp(h)$.

Example 4. As in Examples 2 and 3, let *f* be the monotone decreasing RCTP defined by

$$f(\theta) = 1 + 24\cos\theta - 12\cos(2\theta) + 8\cos(3\theta)$$
$$-3\cos(4\theta).$$

Suppose we are interested in the *j*th largest eigenvalue $\lambda_j(T_n(f))$ for (j, n + 1) = (100, 1000). Note that *n* is not dramatically large in this case, so we may compute $\lambda_j(T_n(f))$ by a standard eigensolver, thus obtaining

$$\lambda_i(T_n(f)) = 17.89119035373482\dots (3-20)$$

Let us now compute the approximation of $\lambda_j(T_n(f))$ given by Algorithm 1 with $(j_1, n_1 + 1) = (4, 40)$, $(j_2, n_2 + 1) = (5, 50)$, $(j_3, n_3 + 1) = (10, 100)$. We follow the algorithm step by step.

• Due to the small size of n_1 , n_2 , n_3 , the eigenvalues $\lambda_{j_1}(T_{n_1}(f))$, $\lambda_{j_2}(T_{n_2}(f))$, $\lambda_{j_3}(T_{n_3}(f))$ can be efficiently computed by, say, the MATLAB eig function, which yields the values

$$\lambda_{j_1}(T_{n_1}(f)) = 17.86119786677332...$$

$$\lambda_{j_2}(T_{n_2}(f)) = 17.86764984932256...$$

$$\lambda_{j_3}(T_{n_3}(f)) = 17.88024043750535...$$

In this example we have θ
 = θ_{j,n} = π/10, and the errors E_{j1,n1,0}, E_{j2,n2,0}, E_{j3,n3,0} are given by

$$E_{j_1,n_1,0} = \lambda_{j_1}(T_{n_1}(f)) - f(\bar{\theta})$$

= -0.03118562702593...
$$E_{j_2,n_2,0} = \lambda_{j_2}(T_{n_2}(f)) - f(\bar{\theta})$$

= -0.02473364447669...
$$E_{j_3,n_3,0} = \lambda_{j_3}(T_{n_3}(f)) - f(\bar{\theta})$$

= -0.01214305629390...

Let p(x) be the interpolation polynomial for the data (h₁, E_{j1,n1,0}/h₁), (h₂, E_{j2,n2,0}/h₂), (h₃, E_{j3,n3,0}/h₃). The value p(h) can be computed from the Lagrange form of p(x):

$$p(h) = \frac{E_{j_1,n_1,0}}{h_1} \frac{(h-h_2)(h-h_3)}{(h_1-h_2)(h_1-h_3)} \\ + \frac{E_{j_2,n_2,0}}{h_2} \frac{(h-h_1)(h-h_3)}{(h_2-h_1)(h_2-h_3)} \\ + \frac{E_{j_3,n_3,0}}{h_3} \frac{(h-h_1)(h-h_2)}{(h_3-h_1)(h_3-h_2)} \\ = -1.19315109114712\dots$$

f	$\lambda_j(T_n(f))$	$f(\bar{\theta}) + hp(h)$	Error $\left \lambda_{j}(T_{n}(f)) - f(\bar{\theta}) - hp(h)\right $	Error Estimate $C_3 \left[\sum_{i=1}^3 \hat{a}_i h_i^4 + h^4 \right]$
f_2 f_3	1.07487275461020 1.11519899215300 1.15757222445221	1.07487275470961 1.11519899090697	$9.94 \cdot 10^{-11}$ $1.25 \cdot 10^{-9}$ $4.05 \cdot 10^{-8}$	$C_3 \cdot 9.47 \cdot 10^{-10}$ $C_3 \cdot 9.47 \cdot 10^{-10}$ $C_3 \cdot 0.47 \cdot 10^{-10}$

Table 1. Example 5: Comparison between $\lambda_i(T_n(f))$ and $f(\bar{\theta}) + hp(h)$ for several RCTPs f.

• The approximation of $\lambda_j(T_n(f))$ returned by the algorithm is

$$\lambda_j(T_n(f)) \approx f(\theta) + hp(h) = 17.89119034270811... (3-21)$$

A direct comparison between (3-20) and (3-21)shows that $|\lambda_j(T_n(f)) - f(\bar{\theta}) - hp(h)| \approx 1.10 \cdot 10^{-8}$ (!). Assuming we have no information about the exact value (3-20), we can estimate the error $|\lambda_j(T_n(f)) - f(\bar{\theta}) - hp(h)|$ via (3-19). The coefficients $\hat{a}_1, \hat{a}_2, \hat{a}_3$ are easily computed by solving the linear system (3-17), which in this case becomes

$$\begin{bmatrix} h_1 & h_2 & h_3 \\ h_1^2 & h_2^2 & h_3^2 \\ h_1^3 & h_2^3 & h_3^3 \end{bmatrix} \begin{bmatrix} \hat{a}_1 \\ \hat{a}_2 \\ \hat{a}_3 \end{bmatrix} = \begin{bmatrix} h \\ h^2 \\ h^3 \end{bmatrix}$$
$$\iff \begin{bmatrix} \hat{a}_1 \\ \hat{a}_2 \\ \hat{a}_3 \end{bmatrix} = \begin{bmatrix} 0.0912 \\ -0.216 \\ 0.304 \end{bmatrix}.$$

By (3-19),

$$|\lambda_j(T_n(f)) - f(\bar{\theta}) - hp(h)| \le C_3 \cdot 7.33 \cdot 10^{-8}$$

where C_3 is a constant depending only on f.

Example 5. In this example, for several RCTPs f and for the fixed pair (j, n) = (1700, 5000), we compare $\lambda_j(T_n(f))$ to its approximation $f(\bar{\theta}) + hp(h)$ provided by Algorithm 1 with $(j_1, n_1 + 1) = (17, 50)$, $(j_2, n_2 + 1) = (34, 100)$, $(j_3, n_3 + 1) = (68, 200)$. The results of this comparison are collected in Table 1 for $f = f_q$ and q = 2, 3, 4, where f_q is defined in (1–2). Note that the error estimate in the last column seems to be the same in all cases, but it must be recalled that the constant C_3 depends on f.

4. Numerical experiments and a conjecture for the non-monotone case

Consider the non-monotone RCTP $f(\theta) = 2 + 2\cos\theta - 2\cos(2\theta)$, whose graph over $[0, \pi]$ is depicted in Figure 4. Note that f restricted to the interval $I = (2\pi/3, \pi]$ is monotone and $f^{-1}(f(I)) = I$, where $f(I) = \{f(\theta) : \theta \in I\} = [-2, 2)$ and $f^{-1}(f(I)) = \{\theta \in [0, \pi] : f(\theta) \in f(I)\}$. Let $\lambda_1(T_n(f)), \ldots, \lambda_n(T_n(f))$ be the eigenvalues of $T_n(f)$ arranged in non-decreasing order, and let σ_n be a permutation of $\{1, \ldots, n\}$ which sorts the samples $f(\theta_{1,n}), \ldots, f(\theta_{n,n})$ in nondecreasing order, i.e., $f(\theta_{\sigma_n(1),n}) \leq \cdots \leq f(\theta_{\sigma_n(n),n})$. Note that the inverse permutation $\rho_n = \sigma_n^{-1}$ is supposed to sort the eigenvalues $\lambda_1(T_n(f)), \ldots, \lambda_n(T_n(f))$ so that they match the samples $f(\theta_{1,n}), \ldots, f(\theta_{n,n})$, i.e., $\lambda_{\rho_n(j)}(T_n(f))$ should be approximately equal to $f(\theta_{j,n})$ for all $j = 1, \ldots, n$. In Figure 5 we plot the errors

$$E_{j,n,0} = \lambda_{\rho_n(j)}(T_n(f)) - f(\theta_{j,n})$$
 (4-22)

and the scaled errors $E_{j,n,0}/h$ versus $\theta_{j,n}$ for j = 1, ..., nand n = 100, 200, 400. The fundamental observation is that, as long as $\theta_{j,n} \in I$, the errors $E_{j,n,0}$ draw a smooth curve and the scaled errors $E_{j,n,0}/h$ overlap perfectly, just as in the case of monotone RCTPs (see Figures 1 and 2). We may therefore conjecture that the asymptotic expansion (1–1) holds for the eigenvalues of $T_n(f)$ corresponding in (4–22) to the samples $f(\theta_{j,n})$ with $\theta_{j,n} \in I$. These are essentially the eigenvalues belonging to f(I) = [-2, 2). The precise statement of our conjecture is reported below along with a further example supporting it.

Conjecture 1. Let *f* be an RCTP such that *f* restricted to the interval $I \subseteq [0, \pi]$ is monotone and $f^{-1}(f(I)) = I$. Then, for every integer $\alpha \ge 0$, every *n* and every j = 1, ..., n such that $\theta_{j,n} \in I$, the following asymptotic expansion holds:

$$\lambda_{\rho_n(j)}(T_n(f)) = f(\theta_{j,n}) + \sum_{k=1}^{\alpha} c_k(\theta_{j,n})h^k + E_{j,n,\alpha},$$
(4-23)

where:



Figure 4. Graph of $f(\theta) = 2 + 2\cos\theta - 2\cos(2\theta)$ over $[0, \pi]$.



Figure 5. Errors $E_{j,n,0}$ and scaled errors $E_{j,n,0}/h$ versus $\theta_{j,n}$ for j = 1, ..., n and n = 100, 200, 400 in the case of the symbol $f(\theta) =$ $2+2\cos\theta-2\cos(2\theta)$.



Figure 6. Example 6: Graph of $f(\theta) = 2 - \cos \theta - \cos(3\theta)$ over $[0, \pi].$

- The eigenvalues of $T_n(f)$ are arranged in nondecreasing order, $\lambda_1(T_n(f)) \leq \cdots \leq \lambda_n(T_n(f))$.
- $\rho_n = \sigma_n^{-1}$, where σ_n is a permutation of $\{1, \ldots, n\}$ such that $f(\theta_{\sigma_n(1),n}) \leq \cdots \leq f(\theta_{\sigma_n(n),n})$.
- $\{c_k\}_{k=1,2,...}$ is a sequence of functions from I to \mathbb{R} which depends only on f.
- $h = \frac{1}{n+1}$ and $\theta_{j,n} = \frac{j\pi}{n+1} = j\pi h$. $E_{j,n,\alpha} = O(h^{\alpha+1})$ is the error, which satisfies the inequality $|E_{j,n,\alpha}| \leq C_{\alpha} h^{\alpha+1}$ for some constant C_{α} depending only on α and f.

For $\alpha = 0$, this conjecture is the same as Bogoya, Böttcher, Grudsky, and Maximenko's result (1-3).

Example 6. Let

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

The graph of f is depicted in Figure 6. The hypotheses of Conjecture 1 are satisfied with either $I = [0, \theta)$ or I =



 $(\pi - \hat{\theta}, \pi]$, where $\hat{\theta} = 0.61547970867038...$ To fix the ideas, let $I = [0, \hat{\theta})$. Conjecture 1 with $\alpha = 1$ would say that, for every *n* and every j = 1, ..., n such that $\theta_{i,n} \in I$,

$$\lambda_{\rho_n(j)}(T_n(f)) - f(\theta_{j,n}) = E_{j,n,0} = c_1(\theta_{j,n}) + E_{j,n,1},$$

where $|E_{i,n,1}| \leq C_1 h^2$ and both the function $c_1: I \to \mathbb{R}$ and the constant C_1 depend only on f. In particular, the scaled errors $E_{j,n,0}/h$ corresponding to the points $\theta_{j,n}$ in I should be equal to the equispaced samples $c_1(\theta_{i,n})$ (and should therefore reproduce the graph of c_1) in the limit where $n \to \infty$. In Figure 7 we plot the errors and the scaled errors versus $\theta_{j,n}$ for j = 1, ..., n and n =100, 200, 400. Clearly, the scaled errors overlap perfectly over I, thus supporting Conjecture 1. We remark that nothing would have changed in the reasoning if we had chosen $I = (\pi - \theta, \pi]$.

Assuming Conjecture 1, we can follow the derivation of Section 3 to work out an algorithm, analogous to Algorithm 1, for computing a high precision approximation of $\lambda_{\rho_n(j)}(T_n(f))$ from $\lambda_{\rho_{n_1}(j_1)}(T_{n_1}(f)), \ldots,$ $\lambda_{\rho_{n_m}(j_m)}(T_{n_m}(f))$, provided the corresponding point $\theta_{j_1,n_1} = \cdots = \theta_{j_m,n_m} = \theta_{j,n} = \overline{\theta}$ belongs to an interval $I \subseteq [0, \pi]$ such that $f_{|I|}$ is monotone and $f^{-1}(f(I)) = I$. We report here the algorithm for the reader's convenience.

Algorithm 2. With the notation of this article, given fand m + 1 pairs $(j_1, n_1), \ldots, (j_m, n_m), (j, n)$ such that $j_1h_1 = \cdots = j_mh_m = jh$, we compute a high precision approximation of $\lambda_{\rho_n(j)}(T_n(f))$ as follows:



Figure 7. Example 6: Errors $E_{j,n,0}$ and scaled errors $E_{j,n,0}/h$ versus $\theta_{j,n}$ for j = 1, ..., n and n = 100, 200, 400 in the case of the symbol $f(\theta) = 2 - \cos \theta - \cos(3\theta).$

Table 2. Example 7: Comparison between $\lambda_i(T_n(f))$ and $f(\bar{\theta}) + hp(h)$ for m = 1, ..., 5.

- Compute the eigenvalues $\lambda_{\rho_{n_1}(j_1)}(T_{n_1}(f)), \ldots, \lambda_{\rho_{n_m}(j_m)}(T_{n_m}(f))$ using a standard eigensolver.
- Compute the errors $E_{j_i,n_i,0} = \lambda_{\rho_{n_i}(j_i)}(T_{n_i}(f)) f(\bar{\theta})$ for i = 1, ..., m, where $\bar{\theta} = \theta_{j,n} = j\pi h$.
- Compute p(h), where p(x) is the interpolation polynomial for the data $(h_i, E_{j_i, n_i, 0}/h_i), i = 1, ..., m$.
- Return $f(\theta) + hp(h)$.

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Example 7. Let f be the same as in Example 6. Suppose we are interested in the *j*th smallest eigenvalue $\lambda_j(T_n(f))$ for (j, n+1) = (1000, 10000). The point $\bar{\theta} = \theta_{j,n} = \pi/10$ lies in $I = [0, \hat{\theta}), f_{|I|}$ is monotone and $f^{-1}(f(I)) = I$ (see Figure 6). Moreover, it is clear that the permutation σ_n which sorts the samples $f(\theta_{1,n}), \ldots, f(\theta_{n,n})$ in non-decreasing order is such that $\sigma_n(\ell) = \ell$ for all $\ell = 1, 2, ..., \hat{\ell}$, where $\hat{\ell}$ is the first index such that $\theta_{\hat{\ell}+1,n} \geq \hat{\theta}$. As a consequence, $\rho_n(j) = j$. In Table 2 we compare $\lambda_j(T_n(f))$ to its approximations $f(\theta) + hp(h)$ provided by Algorithm 2 with m = 1, ..., 5 and $(j_1, n_1 + 1) = (3, 30)$, $(j_2, n_2 + 1) = (5, 50), (j_3, n_3 + 1) = (7, 70), (j_4, n_4 + 1)$ 1) = (9, 90), $(j_5, n_5 + 1) = (11, 110)$. Note that, for the same reasoning as above, $\rho_{n_m}(j_m) = j_m$ for all m =1, . . . , 5.

5. Conclusions and perspectives

After supporting through numerical experiments the conjecture that the higher-order approximation (1–1) holds for all monotone RCTPs f, we illustrated how (1–1) can be used along with an extrapolation procedure to compute high precision approximations of the eigenvalues of $T_n(f)$ for large n. Moreover, based on numerical experiments, we formulated a conjecture on the eigenvalue asymptotics of $T_n(f)$ in the case where f is non-monotone, and we showed how the conjecture can be used, again in combination with an extrapolation procedure, to compute high precision approximations of some eigenvalues of $T_n(f)$ for large n.

We conclude this work with a list of possible future lines of research.

• Conjecture 1 does not say anything about "fully nonmonotone" symbols such as $f(\theta) = 2 - 2\cos(\omega\theta)$, where $\omega \ge 2$ is an integer. However, based on numerical experiments, it seems that even in this case a "regular" asymptotics is available for the eigenvalues of $T_n(f)$. For more insights into this topic we refer the reader to papers [Barrera and Grudsky 17] and [Ekström and Serra-Capizzano].

- A noteworthy theoretical objective would be to obtain a precise analytic expression for the error of Algorithm 1, namely |λ_j(T_n(f)) f(θ) hp(h)|. A way to achieve this goal could be to exploit the information about the functions c_k provided in [Bogoya et al. 15a, Bogoya et al. 17, Böttcher et al. 10] and follow the steps in the derivation of the analytic expression for the error of Romberg integration [Bauer 61, Bauer et al. 63].
- With any multi-index $n = (n_1, \ldots, n_d) \in \mathbb{N}^d$ and any multivariate matrix-valued function $f: [-\pi, \pi]^d \to \mathbb{C}^{s \times s}$ whose components f_{ij} belong to $L^1([-\pi, \pi]^d)$, we associate the so-called multilevel block Toeplitz matrix $T_n(f)$, which is defined, e.g., in [Tilli 98]. In view of the design of fast extrapolation algorithms for the computation of the eigenvalues, it would be interesting to know whether an asymptotic expansion such as (1–1) or (4–23) holds even for this kind of matrices. Numerical evidence indicates that the answer should be affirmative if

$$f(\theta_1, \dots, \theta_d) = \sum_{i=1}^d f_q(\theta_i), \quad q = 1, 2, \dots$$
 (5-24)

where f_q is given by (1–2). The *d*-variate function f is especially interesting as it arises in the discretization of partial differential equations over *d*-dimensional domains. For this function, however, we do not need any asymptotic expansion to efficiently compute the eigenvalues of $T_n(f)$. Indeed, due to the specific structure of f, it can be shown that

$$T_n(f) = \sum_{i=1}^d I_{n_1} \otimes \cdots \otimes I_{n_{i-1}} \otimes T_{n_i}(f_q)$$
$$\otimes I_{n_{i+1}} \otimes \cdots \otimes I_{n_d},$$

where I_m is the $m \times m$ identity matrix and \otimes denotes the (Kronecker) tensor product of matrices. By the properties of tensor products, the eigenvalues of $T_n(f)$ are given by

$$\lambda_j(T_n(f)) = \sum_{i=1}^d \lambda_{j_i}(T_{n_i}(f_q)),$$

$$1 \le j_1 \le n_1, \dots, 1 \le j_d \le n_d,$$

and their computation reduces to the computation of the eigenvalues of the unilevel Toeplitz matrices $T_m(f_q)$, which can be performed through Algorithm 1. For functions f more general than (5–24), the reduction to the unilevel setting is not possible. In this case, an extrapolation algorithm for the computation of the eigenvalues of $T_n(f)$ should directly rely on the asymptotic expansion, and establishing whether the latter exists or not is an interesting subject for future research.

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