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REVIEW/SURVEY PAPER

Entries of the inverses of large positive definite Toeplitz matrices

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Abstract
This is an expository paper embarking on the asymptotic behavior of the entries of the inverses of positive definite symmetric Toeplitz matrices as the matrix dimension goes to infinity. We consider the behavior of the entries in neighborhoods of the four corners as well as the density of the distribution of the entries over all of the inverse matrix.

Keywords Toeplitz matrix · Random walk · Green's function

Mathematics Subject Classification Primary 47B35 · Secondary 15B05 · 34B27 · 60G50

1 Introduction

Gabor Szegő's two papers [20] of 1920 and 1921 contain the roots of an enormous development that is lasting until the present. This development includes Toeplitz determinants and orthogonal polynomials, and now there are many recent works which present these topics in expository style; see, for example [4, 7, 18]. Another aspect of Szegő's two papers concerns the analysis of positive definite Toeplitz matrices, and as I am not aware of an expository article devoted exclusively to this issue, I decided to write this paper when receiving the honorable invitation to submit a contribution to the 100th anniversary of the journal Acta Scientiarum Mathematicarum, which was founded by Szegő's contemporaries Alfréd Haar and Frigyes Riesz in 1922

Given a real-valued function a in L^1 over the complex unit circle $\mathbb{T}$, we denote by $a_k = \int_{-\pi}^{\pi} a(e^{i\theta})e^{-ik\theta}\, d\theta/(2\pi)$ $(k \in \mathbb{Z})$ its Fourier coefficients and by $T_n(a)$ the $n \times n$ Toeplitz matrix

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$$T_n(a) = (a_{j-k})_{j,k=1}^n = \begin{pmatrix} a_0 & a_{-1} & \dots & a_{-(n-1)} \\ a_1 & a_0 & \dots & a_{-(n-2)} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n-1} & a_{n-2} & \dots & a_0 \end{pmatrix}.$$

Since a is real-valued, this matrix is Hermitian. We confine ourselves to the case where the matrix is real and thus symmetric. This is equivalent to the requirement that the function $\theta \mapsto a(e^{i\theta})$ is even on $(-\pi, \pi)$. If $a \geq 0$ almost everywhere on $\mathbb{T}$ and a is not identically zero, then $T_n(a)$ is positive definite. Indeed, if $x = (x_0, \dots, x_{n-1})^\top \in \mathbb{C}^n$, then

$$(T_n(a)x, x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} a(e^{i\theta}) |x(e^{i\theta})|^2 \, d\theta \tag{1}$$

with $x(e^{i\theta}) = x_0 + x_1 e^{i\theta} + \dots + x_{n-1} e^{i(n-1)\theta}$, and the integral is clearly strictly positive.

Throughout this paper we assume that $a \in L^1$ is real-valued and not identically zero, that $a_k = a_{-k}$ for all k, and that $a \geq 0$ a.e. on $\mathbb{T}$, so that $T_n(a)$ is (symmetric) positive definite and hence invertible for all $n \geq 1$. We are interested in the entries of the inverse matrix $T_n^{-1}(a) := [T_n(a)]^{-1}$.

The interest in the entries of the inverse is, for example, motivated by the following result of Spitzer and Stone [19] on random walks with deadly barriers. Let $\{h_k\}_{k=-\infty}^{\infty}$ be a sequence of non-negative numbers such that

$$h_k = h_{-k} \quad \text{for all} \quad k, \qquad \sum_{k=-\infty}^{\infty} h_k = 1, \qquad 0 < \sum_{k=-\infty}^{\infty} k^2 h_k = \sigma^2 < \infty,$$

and g.c.d.$\{k : h_k > 0\} = 1$. Put $a(t) = 1 - \sum_{k=-\infty}^{\infty} h_k t^k$ for $t = e^{i\theta} \in \mathbb{T}$. Clearly, $a \geq 0$ on $\mathbb{T}$. Let X be a random variable that assumes the value k with probability h_k, that is, $\mathbb{P}(X = k) = h_k$. With an unspecified integer S_0, consider the stochastic process

$$S_n = S_0 + X_1 + X_2 + \dots + X_n \quad (n \geq 1),$$

where the X_i are identically distributed, independent copies of X. Then

$$[T_n^{-1}(a)]_{j,k} = \sum_{\ell=0}^{\infty} \mathbb{P}\left[S_\ell = k \ \text{ and } \ 1 \leq S_i \leq n \ \text{ for } \ i = 0, 1, \dots, \ell \,|S_0 = j\right].$$

Equivalently, $[T_n^{-1}(a)]_{j,k}$ is the expected number of visits of the stochastic process S_n to the point k starting with $S_0 = j$ and before leaving the closed interval $[1, n]$ for the first time. In the case where $h_1 = h_{-1} = 1/2$ and $h_k = 0$ for all other k, this insight was already gained by Courant, Friedrichs, and Lewy in [6]. In this special case the matrix $T_n(a)$ is the tridiagonal Toeplitz matrix

$$T_n(a) = \begin{pmatrix} 1 & -1/2 & 0 & \dots & 0 \\ -1/2 & 1 & -1/2 & \dots & 0 \\ 0 & -1/2 & 1 & \dots & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & 0 & 0 & \dots & 1 \end{pmatrix}_{n\times n}. \tag{2}$$

This is 1/2 times the matrix we will examine in Sect. 2.

There are clever fast and stable algorithms for solving systems with positive definite Toeplitz matrices and thus for inverting such matrices. These give the desired entries within seconds for n up to some thousands. However, if a depends on a parameter or if one wants to know the behavior of the entries for $n \to \infty$, one cannot invoke numerical algorithms. The purpose of this paper is to record a couple of (mostly known) tools that can be employed to tackle such problems.

One well-known and very useful tool is the Gohberg–Sementsul–Trench formula [10, 22]. Full proofs can also be found in [9, Chap. III.6.1] and [11, p. 21]. In the case of positive definite symmetric matrices, it says that if $(c_1\ c_2\ \dots\ c_n)^\top$ is the first column of $T_n^{-1}(a)$ or, equivalently, the solution of the system $T_n(a)c = e_1$ with $e_1 = (1\ 0\ \dots\ 0)^\top$, then $c_1 \neq 0$ and

$$\begin{aligned} T_n^{-1}(a) = &\frac{1}{c_1}\begin{pmatrix} c_1 & & & \\ c_2 & c_1 & & \\ \vdots & \vdots & \ddots & \\ c_n & c_{n-1} & \dots & c_1 \end{pmatrix}\begin{pmatrix} c_1 & c_2 & \dots & c_n \\ & c_1 & \dots & c_{n-1} \\ & & \ddots & \vdots \\ & & & c_1 \end{pmatrix} \\ &- \frac{1}{c_1}\begin{pmatrix} 0 & & & & \\ c_n & 0 & & & \\ c_{n-1} & c_n & 0 & & \\ \vdots & \vdots & \ddots & & \\ c_2 & c_3 & \dots & c_n & 0 \end{pmatrix}\begin{pmatrix} 0 & c_n & c_{n-1} & \dots & c_2 \\ & 0 & c_n & \dots & c_3 \\ & & & \ddots & \vdots \\ & & & & c_n \\ & & & & 0 \end{pmatrix}. \end{aligned} \tag{3}$$

Thus, the entire inverse matrix is captured in its first column. Note also that Cramer's rule gives $c_1 = \det T_{n-1}(a)/ \det T_n(a)$.

2 An illuminating example

Let $\alpha \in \mathbb{R}$ and consider $a(t) = -t + \alpha - t$ for $t = e^{i\theta} \in \mathbb{T}$. The Fourier coefficients of a are $a_0 = \alpha$, $a_1 = a_{-1} = -1$, and $a_k = 0$ for $|k| \geq 2$. The matrix $T_n(a)$ is the $n \times n$ tridiagonal symmetric Toeplitz matrix with 2 on the main diagonal and -1 on the subdiagonal and the superdiagonal. We have $a \geq 0$ on $\mathbb{T}$ if and only if $\alpha \geq 2$. Thus, for $\alpha \geq 2$, the matrix $T_n(a)$ is positive definite and hence invertible. We write $T_n^{-1}(a) = (c_{jk}^{(n)})_{j,k=1}^n$ and so have (3) with c_j replaced by $c_j^{(n)} = c_{j,1}^{(n)}$.

Let first $\alpha = 2$, that is, consider the case where $T_n(a)$ is 2 times the matrix (2). The reader is invited to try

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inv(toeplitz([2 −1 zeros(1,n − 2)]))
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for $n = 8$ and $n = 9$ in Matlab to see that these two inverses are particular beauties. It is a standard exercise to show that $\det T_n(a) = n + 1$ for $n \geq 1$, which gives $c_1^{(n)} = n/(n+1)$. The equations of the system $T_n(a)c = e_1$ are

$$2c_1^{(n)} - c_2^{(n)} = 1, \quad -c_1^{(n)} + 2c_2^{(n)} - c_3^{(n)} = 0, \quad \dots, \quad 2c_{n-1}^{(n)} - c_n^{(n)} = 0$$

and as $c_1^{(n)}$ is known, these equations successively yield

$$c_2^{(n)} = \frac{n-1}{n+1}, \quad c_3^{(n)} = \frac{n-2}{n+1}, \quad \dots, \quad c_n^{(n)} = \frac{1}{n+1}. \tag{4}$$

Consequently, $c_j^{(n)} \to 1$ and $c_{n+1-j}^{(n)} \to 0$ as $n \to \infty$ for each fixed j. It follows from (3) that the upper left corner of the matrix $T_n^{-1}(a)$ approaches

$$\begin{pmatrix} 1 & 1 & 1 & 1 & \dots \\ 1 & 2 & 2 & 2 & \dots \\ 1 & 2 & 3 & 3 & \dots \\ 1 & 2 & 3 & 4 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \tag{5}$$

as $n \to \infty$. In other terms, for each fixed m, the upper-left $m \times m$ corner of $T_n^{-1}(a)$ converges to $(\min(j,k))_{j,k=1}^m$ as $n \to \infty$. By symmetry, the limit of the lower-right corner is the double flip of this matrix. Analogously one obtains that that the upper-right and lower-left corners of $T_n^{-1}(a)$ approach the zero matrix as $n \to \infty$.

Once $c_1^{(n)}, \dots, c_n^{(n)}$ are available, formula (3) allows us to determine the j, k entry of the inverse by elementary computations. For example, the k, k entry turns out to be $k(n+1-k)/(n+1)$, which is about $n/4$ for k around $n/2$. The left picture of Fig. 1 shows a pseudocolor plot of $T_{100}^{-1}(a)$. One suspects that after shrinking the inverse to the square $Q = [0,1]^2$, the appropriately scaled values of the entries will eventually form a nice surface about Q. To be more precise, the expectation is that after changing the enumeration of the entries from $1, 2, \dots, n$ to $0, 1, \dots, n-1$ and denoting by $[\varrho]$ the integral part of $\varrho \in \mathbb{R}$, one has

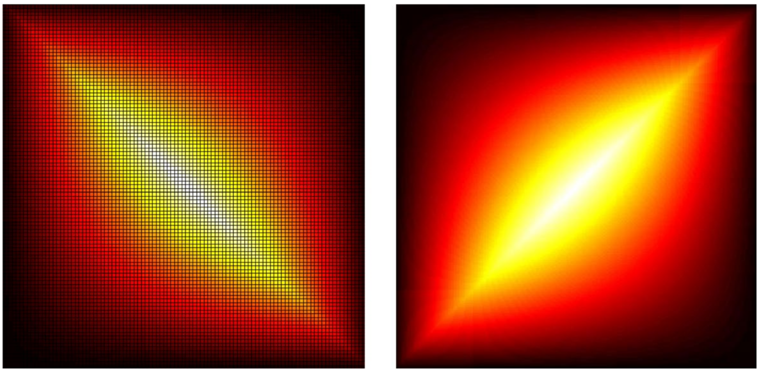

Fig. 1 Pseudocolor plots of the inverse matrix (left) and of $G(x, y)$ (right) in the case where $\alpha = 2$

$$[T_n^{-1}(a)]_{[nx],[ny]} = G(x,y)n + O(1) \quad \text{as} \quad n \to \infty$$

with some function $G : Q \to \mathbb{R}$ which is given on the diagonal $x = 1 - y$ of Q by $G(x,x) = x(1-x)$. This can indeed be proved by simply computing the j, k entry using (3) and (4). It results that G is symmetric about the diagonals $x = y$ and $x = 1 - y$ and that $G(x,y) = x(1-y)$ for $0 \le x \le y \le 1$. In the right picture of Fig. 1 we see a pseudocolor plot of G. The two pictures fit after a flip about the horizontal axis (because the rows of a matrix are numbered downwards, whereas the y-axis of Q is oriented upwards).

Now let $\alpha > 2$. In that case things change drastically. For $f \in L^1$, we denote by $T(f)$ the infinite Toeplitz matrix $(f_{j-k})_{j,k=1}^{\infty}$. If even $f \in L^\infty$, this matrix induces a bounded linear operator on $\ell^2(\mathbb{N})$ in the natural fashion. If $\alpha = 2$, the operator $T(a)$ is not (boundedly) invertible: its formal inverse is given by the extension of (5) to an infinite matrix, and this matrix does clearly not generate a bounded operator. However, if $\alpha > 2$, then $T(a)$ has a bounded inverse, denoted by $T^{-1}(a) := [T(a)]^{-1}$. This inverse can be found by what is called Wiener–Hopf factorization. Recall that $t = e^{i\theta} \in \mathbb{T}$. Simple computation shows that

$$a(t) = -t^{-1} + \alpha - t = \frac{1}{\gamma}\left(1 - \frac{\gamma}{t}\right)(1 - \gamma t)$$

with $\gamma = \alpha/2 - \sqrt{\alpha^2/4 - 1} \in (0,1)$. Putting

$$a_-(t) = 1 - \gamma/t, \quad a_+(t) = (1/\gamma)(1 - \gamma t),$$

we get the Wiener–Hopf factorization $a = a_- a_+$, and the inverse $T^{-1}(a)$ can be shown to be $T(a_+^{-1})T(a_-^{-1})$; see, for example, [4, Sect. 1.5]. We have the Fourier expansions

$$a_+^{-1}(t) = \gamma(1 + \gamma t + \gamma^2 t^2 + \cdots), \quad a_-^{-1}(t) = 1 + \gamma t^{-1} + \gamma^2 t^{-2} + \cdots,$$
$$a^{-1}(t) = a_+^{-1}(t)a_-^{-1}(t) = \frac{\gamma}{1-\gamma^2}(\cdots + \gamma^2 t^{-2} + \gamma t^{-1} + 1 + \gamma t + \gamma^2 t^2 + \cdots).$$

The expansions for $a_\pm^{-1}$ give

$$T^{-1}(a) = \frac{\gamma}{1-\gamma^2}\begin{pmatrix} 1-\gamma^2 & \gamma(1-\gamma^2) & \gamma^2(1-\gamma^2) & \gamma^3(1-\gamma^2) & \dots \\ \gamma(1-\gamma^2) & 1-\gamma^4 & \gamma(1-\gamma^4) & \gamma^2(1-\gamma^4) & \dots \\ \gamma^2(1-\gamma^2) & \gamma(1-\gamma^4) & 1-\gamma^6 & \gamma(1-\gamma^6) & \dots \\ \gamma^3(1-\gamma^2) & \gamma^2(1-\gamma^4) & \gamma(1-\gamma^6) & 1-\gamma^8 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}. \tag{6}$$

A formula by Widom [24] (which is as Theorem 2.14 also in [4]) reads

$$T_n^{-1}(a) = P_n T^{-1}(a) P_n + W_n K(a) W_n + C_n \tag{7}$$

$$= T_n(a^{-1}) + P_n K(a) P_n + W_n K(a) W_n + C_n \tag{8}$$

where P_n is projection onto the first n coordinates, W_n is P_n followed by reversal of the coordinates, $K(a) = T^{-1}(a) - T(a^{-1})$, and $\|C_n\| \to 0$ as $n \to \infty$. Here $P_n A P_n : \ell^2(\mathbb{N}) \to \ell^2(\mathbb{N})$ is identified with an $n \times n$ matrix in the obvious manner. From (6) and the Fourier expansion of a^{-1} we obtain

$$K(a) = -\frac{\gamma^2}{1-\gamma^2}\begin{pmatrix} \gamma & \gamma^2 & \gamma^3 & \dots \\ \gamma^2 & \gamma^3 & \gamma^4 & \dots \\ \gamma^3 & \gamma^4 & \gamma^5 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}.$$

The (Hankel) operator $K(a)$ is compact, W_n converges weakly to zero, and P_n converges strongly to the identity operator. It follows in particular that $W_n K(a) W_n$ converges strongly to zero and thus (7) tells us that, for each fixed $m \geq 1$, the upper-left $m \times m$ corner of $T_n^{-1}(a)$ converges to the upper-left $m \times m$ corner of the infinite matrix (6). The lower-right corner of $T_n^{-1}(a)$ is simply the double flip of the upper-left one. Finally, since the upper-right and lower-left corners of $P_n T^{-1}(a) P_n$ converge to zero, so do by virtue of (8) also the upper-right and lower-left corners of $T_n^{-1}(a)$.

What about the overall distribution of the values of the entries of $T_n^{-1}(a)$ when shrinking the matrix to the square $Q = [0,1]^2$? Recall that $K(a)$ is compact and that hence its main mass is concentrated near the upper-left corner. It follows that as n increases, the main mass of the shrunk matrices $P_n K(a) P_n$ and $W_n K(a) W_n$ is in pieces that become smaller and smaller and throng in the upper-left and lower-right corners of the (flipped) unit square, respectively. From (8) we therefore obtain that

$$[T_n^{-1}(a)]_{[nx],[ny]} = (a^{-1})_{[nx]-[ny]} + o(1) \quad \text{for} \quad (x,y) \in Q \backslash \{(0,0),(1,1)\}$$

as $n \to \infty$. Thus, letting Δ denote the diagonal $x = y$ of Q, we arrive at the following: $[T_n^{-1}(a)]_{[nx],[n,y]}$ converges pointwise to 0 on $Q \backslash \Delta$ and pointwise to $(a^{-1})_0 = \gamma/(1-\gamma^2)$ on $\Delta \backslash \{(0,0),(1,1)\}$, the convergence to 0 is uniform on compact subsets of $Q \backslash \Delta$, and the convergence to $(a^{-1})_0 = \gamma/(1-\gamma^2)$ is uniform on compact subsets of $\Delta \backslash \{(0,0),(1,1)\}$. Finally, combining (6) and (7), we see that $[T_n^{-1}(a)]_{0,0} = [T_n^{-1}(a)]_{n-1,n-1} \to \gamma$. Figure 2 illustrates concrete cases.

3 Convergence of corner entries

We now turn to a fairly large class of functions. Let $a \in L^1 := L^1(\mathbb{T})$, suppose the function $\theta \mapsto a(e^{i\theta})$ is real-valued, non-negative, and even on $(-\pi, \pi)$, and assume $\log a$ is also in L^1. The latter assumption admits polynomial zeros on $\mathbb{T}$, but it rules out functions with strong zeros, in particular functions vanishing identically on entire intervals. Let $\log a(t) = \sum_{k=-\infty}^{\infty} (\log a)_k t^k$ $(t = e^{i\theta} \in \mathbb{T})$ be the Fourier expansion. The Riemann–Lebesgue lemma implies that the coefficients $(\log a)_k$ go to 0 as $|k| \to \infty$. It follows that

$$a_+(z) = \exp \sum_{k=0}^{\infty} (\log a)_k z^k$$

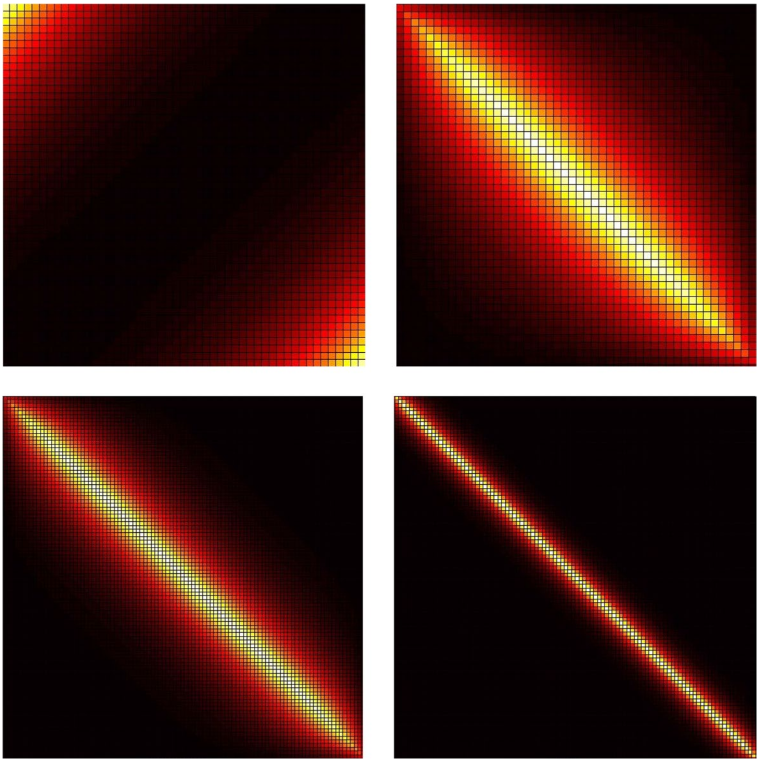

Fig. 2 Pseudocolor plots of $T_n(a^{-1}) - T_n^{-1}(a) \approx P_n(-K(a))P_n + W_n(-K(a))W_n$ (upper left) and of the inverse matrix $T_n^{-1}(a)$ (upper right) for $n = 50$ and $\alpha = 2.01$. Pseudocolor plots of $T_n^{-1}(a)$ for $n = 100$ and $\alpha = 2.01$ (lower left) and for $n = 100$ and $\alpha = 2.1$ (lower right)

is an analytic function in the open unit disk $|z| < 1$. We write

$$a_+^{-1}(z) = \exp\left(-\sum_{k=0}^{\infty} (\log a)_k z^k \right) = \sum_{k=0}^{\infty} (a_+^{-1})_k z^k.$$

Combining the following theorem with formula (3) we arrive at the conclusion that, for each fixed $m \geq 1$, the upper-left and lower-right $m \times m$ principal submatrices of $T_n^{-1}(a)$ converge to certain finite limits and that the $m \times m$ submatrices in upper-right and lower-left corners of $T_n^{-1}(a)$ converge to the zero matrices.

Theorem 1 *Let $c_k^{(n)}$ be the kth component of the first column of $T_n^{-1}(a)$. Then, for each fixed $j \geq 1$,*

$$\lim_{n\to\infty} c_j^{(n)} = (a_+^{-1})_{j-1}, \quad \lim_{n\to\infty} c_{n+1-j}^{(n)} = 0.$$

Various versions of this theorem are known for a long time; see, for example, [19, Theorem 1.6]. In the form presented, that is, under the sole assumption that

$a \in L^1$, $a \geq 0$, $\log a \in L^1$, it was stated with a full proof in [3], but it may well be that this is also known. The polynomials

$$\Phi_{n-1}(z) = \frac{1}{c_1^{(n)}}\left(c_n^{(n)} + c_{n-1}^{(n)} z + \cdots + c_1^{(n)} z^{n-1}\right)$$

are called the Szegő polynomials of a. They are the monic orthogonal polynomials on $\mathbb{T}$ with respect to the measure $a(e^{i\theta})d\theta/(2\pi)$. Theorem 1 is therefore a result on the limiting behavior of the coefficients of these polynomials and its proof is based on the classical results in this field, which can be found in [18, 20, 21]. Notice that $(a_+^{-1})_0 = \exp(-(\log a)_0) = 1/G(a)$, where $G(a) = \exp(\log a)_0$ is the so-called geometric mean of a, and that the convergence

$$c_1^{(n)} = \det T_{n-1}(a)/\det T_n(a) \to 1/G(a)$$

is a classical result of Szegő. We also note that $a_+(z)$ is sometimes defined as

$$a_+(z) = \exp \sum_{k=1}^{\infty} (\log a)_k z^k \quad \text{or} \quad a_+(z) = \exp\left(\frac{(\log a)_0}{2} + \sum_{k=1}^{\infty} (\log a)_k z^k.\right)$$

Then the $(a_+^{-1})_{j-1}$ in Theorem 1 must be replaced by $(1/G(a))(a_+^{-1})_{j-1}$ or $(1/G(a)^{1/2})(a_+^{-1})_{j-1}$. (In Example 5.3 of [3], the factor $1/G(b)$ is correctly contained in the formula for c_j but incorrectly missing in the formulas for c_1, c_2, c_3.)

Example 1 Let $a(t) = |1-t|^{2p}$ where $p \in (-1/2, \infty)$. For $p = 1$, this is the function $2 - t^{-1} - t$ examined in Sect. 2. If $p = 2$, we get the pentadiagonal symmetric Toeplitz matrix whose first row is $(6\ \ -4\ 1\ 0\ \ldots)$. The matrices $T_n(a)$ are no longer banded if $p \notin \mathbb{Z}$. In the case at hand, $a(t) = (1-t^{-1})^p(1-t)^p$, hence

$$\log a(t) = p\log(1-t^{-1}) + p\log(1-t) = -p\sum_{k=1}^{\infty}\frac{t^{-k}}{k} - p\sum_{k=1}^{\infty}\frac{t^k}{k},$$

which shows that $a_+^{-1}(z)$ equals

$$\exp\left(p\sum_{k=1}^{\infty}\frac{z^k}{k}\right) = \exp(-p\log(1-z)) = (1-z)^{-p} = \sum_{j=0}^{\infty}\binom{p+j-1}{j}z^j.$$

Consequently, the limit of $c_j^{(n)}$ is $\binom{p+j-2}{j-1}$. Theorem 4.1 of [3] contains the more precise result

$$c_j^{(n)} = \binom{p+j-2}{j-1}\left(1 - \frac{p(p+1)}{n} + O\left(\frac{1}{n^2}\right)\right) \quad \square$$

To include a more general case, let $a(t) = |1-t|^{2p}b(t)$ where $p \in (-1/2, \infty)$ and b is bounded and bounded away from zero in an open neighborhood of

$t = 1$. Our assumptions on a imply that b and $\log b$ are also in L^1. We now have $a(t) = b(t)(1 - t^{-1})^p(1 - t)^p$, so

$$\log a(t) = \sum_{k=-\infty}^{\infty} (\log b)_k t^k - p \sum_{k=1}^{\infty} \frac{t^{-k}}{k} - p \sum_{k=1}^{\infty} \frac{t^k}{k},$$

it follows that $a_+^{-1}(z)$ is equal to

$$\exp\left(- \sum_{k=0}^{\infty} (\log b)_k z^k + p \sum_{k=1}^{\infty} \frac{z^z}{k} \right) = b_+^{-1}(z)(1 - z)^{-p}$$
$$= \left((b_+^{-1})_0 + (b_+^{-1})_1 z + (b_+^{-1})_2 z^2 + \cdots\right)\left(1 + \binom{p}{1} z + \binom{p+1}{2} z^2 + \cdots\right)$$

and eventually we obtain $c_1^{(n)} \to (b_+^{-1})_0$, $c_2^{(n)} \to (b_+^{-1})_0 \binom{p}{1} + (b_+^{-1})_1$, etc.

Example 2 Let $T_n(a)$ be the pentadiagonal symmetric Toeplitz matrix whose first row is $(4\ \ -1\ \ -1\ 0\ \ \ldots)$. Clearly, $a = 4 - t - t^{-1} - t^2 - t^{-2} \geq 0$ for $t \in \mathbb{T}$. We have $a(t) = (1 - t)(1 - t^{-1})(3 + t - t^{-1})$ and may write

$$a(t) = |1 - t|^2 \left(1 - \frac{\delta}{t}\right)(t - \gamma) \quad \text{with} \quad \gamma = \frac{-3 - \sqrt{5}}{2}, \ \ \delta = \frac{-3 + \sqrt{5}}{2}.$$

Thus, with $b_+(z) = z - \gamma = -\gamma(1 - z/\gamma)$ we obtain that the limit c_j of $c_j^{(n)}$ equals

$$c_j = -\frac{1}{\gamma}[(1 - z)^{-1} b_+^{-1}(z)]_{j-1} = -\frac{1}{\gamma}\left[\left(1 + z + z^2 + \cdots\right)\left(1 + \frac{z}{\gamma} + \frac{z^2}{\gamma^2} + \cdots\right)\right]_{j-1}.$$

What results is

$$c_1 = -\frac{1}{\gamma}, \quad c_2 = -\frac{1}{\gamma}\left(\frac{1}{\gamma} + 1\right), \quad c_3 = -\frac{1}{\gamma}\left(\frac{1}{\gamma^2} + \frac{1}{\gamma} + 1\right), \quad \ldots.$$

Inserting $\gamma = (-3 - \sqrt{5})/2$ and using (3) we see after some computations that the upper-left 3×3 corner of $T_n^{-1}(a)$ converges to

$$\begin{pmatrix} 3/2 - (1/2)\sqrt{5} & \sqrt{5} - 2 & 7 - 3\sqrt{5} \\ \sqrt{5} - 2 & 5 - 2\sqrt{5} & 6\sqrt{5} - 13 \\ 7 - 3\sqrt{5} & 6\sqrt{5} - 13 & 18\sqrt{5} - 41 \end{pmatrix}. \ \square$$

In the case where a is not only non-negative on $\mathbb{T}$ but even bounded and bounded away from zero (which is the case $\alpha > 2$ in Sect. 2), a little more can be said. So suppose a is actually a real-valued and even function in L^∞ and there is an $\varepsilon > 0$ such that $a \geq \varepsilon$ a.e. on $\mathbb{T}$. Then the infinite Toeplitz matrix $T(a)$ induces a bounded and invertible operator on $\ell^2(\mathbb{N})$. We may the matrices $T_n(a)$ identify with the operator $P_n T(a) P_n$, and this operator converges strongly to $T(a)$. From (1) we infer that the eigenvalues of $T_n(a)$ are all greater than or equal to $\varepsilon > 0$, which reveals that the norms of the inverses

$T_n^{-1}(a)$ are uniformly bounded for $n \geq 1$. All this together implies that the so-called finite section method is applicable to $T(a)$, which means that $T_n^{-1}(a)P_n = (P_n T(a) P_n)^{-1} P_n$ converges strongly to $T^{-1}(a)$; see, e.g., [4, Sect. 2.1] or [9, Chap. II.2]. It follows in particular from Theorem 1 that $\{c_j\}_{j=1}^{\infty}$ with $c_j = (a_+^{-1})_{j-1}$ is the sequence of entries of the first column of $T^{-1}(a)$ and that not only $c_j^{(n)} \to c_j$ but even $\|T_n^{-1}(a)P_n e_1 - T^{-1}(a)e_1\| \to 0$, that is, $\sum_{j=1}^{n} |c_j^{(n)} - c_j|^2 \to 0$ as $n \to \infty$.

4 Global limiting distribution

The subject of this section is the behavior of $[T_n^{-1}(a)]_{[nx],[ny]}$ for $(x, y) \in Q = [0, 1]^2$ as $n \to \infty$. Recall that in this context we number rows and columns from 0 to $n - 1$ and not from 1 to n.

If a takes positive values, is continuous, and bounded away from zero on $\mathbb{T}$, then $T(a)$ is invertible and Widom's formulas (7) and (8) hold with compact $K(a)$ and with $\|C_n\| \to 0$. Thus, Fig. 2 describes the typical picture for $T_n^{-1}(a)$ also in this general situation. The function $[T_n^{-1}(a)]_{[nx],[ny]}$ converges pointwise to zero on $Q \setminus \Delta$, where Δ is the diagonal $x = y$, and pointwise to $(a^{-1})_0$ on $\Delta \setminus \{(0, 0), (1, 1)\}$, the convergences being uniform on compact subsets of $Q \setminus \Delta$ and $\Delta \setminus \{(0, 0), (1, 1)\}$.

Things become more interesting if a has zeros on $\mathbb{T}$. Throughout this section we assume that $a(t) = |1 - t|^{2p} b(t)$ with an integer $p \geq 1$ and with a continuous function $b : \mathbb{T} \to [\varepsilon, \infty)$ $(\varepsilon > 0)$ whose Fourier coefficients satisfy $b_k = b_{-k}$ for all k and $\sum_{k=-\infty}^{\infty} |k||b_k| < \infty$. Paper [16] treats the case where p is no longer assumed to be an integer. The following result is the Theorema Egregium in the business.

Theorem 2 *We have, uniformly in* $(x, y) \in Q$,

$$[T_n^{-1}(a)]_{[nx],[ny]} = \frac{1}{b(1)} G_p(x, y) n^{2p-1} + o(n^{2p-1})$$

with some $G_p(x, y)$ *independent of* b.

This theorem was explicitly established by Rambour and Seghier in [14]. See also [15], where [1] is already incorporated. For $p = 1$, a result of this type was known from the classics [6, 19] and also from [13] with $G_1(x, y) = \min(x, y) - xy$, which is Green's function associated with the second derivative operator on [0, 1]. Section 2 is about $p = 1$ and the case where b is identically 1; the $G(x, y)$ we encountered there is nothing but $G_1(x, y)$. The function $G_p(x, y)$ is symmetric about the diagonals $x = y$ and $x = 1 - y$, and hence it suffices to find it for $0 \leq x \leq y \leq 1$ or even only for $0 \leq x \leq 1$ and $y \geq \max(x, 1 - x)$. Rambour and Seghier [14] derived formulas that allow us to compute at least in principle $G_p(x, y)$ recursively and showed that

$$G_2(x, y) = \frac{1}{6} x^2 (1 - y)^2 (3y - x - 2xy) \quad \text{for} \quad 0 \leq x \leq y \leq 1.$$

The following expression for $G_p(x, y)$ was established in [1].

Theorem 3 *For* $0 \le x \le 1$ *and* $y \ge \max(x, 1-x)$,

$$G_p(x,y) = \frac{x^p y^p}{[(p-1)!]^2} \int_y^1 \frac{(t-x)^{p-1}(t-y)^{p-1}}{t^{2p}}\, dt.$$

The proof of this theorem is based on the independence of $G_p(x,y)$ of b, which implies that we need to compute $G_p(x,y)$ only for the pure singularity $\omega_p(t) = |1-t|^{2p}$. This can be done with the help of a formula by Duduchava [8] and Roch [17]. Paper [2] contains the formula together with a full proof, the story behind it, and several of its applications. For $0 \le j \le k \le n-1$, the Duduchava-Roch formula gives

$$[T_n^{-1}(\omega_p)]_{j,k} = \frac{\binom{j+p}{p}\binom{k+p}{p}}{\binom{2p}{p}} \sum_{\ell=k}^{n-1} \frac{\binom{\ell-j+p-1}{p-1}\binom{\ell-k+p-1}{p-1}}{\binom{\ell+2p}{p}},$$

and Theorem 3 results from this formula by letting $j=[nx], k=[ny]$ and performing some analysis. The integral in Theorem 3 can be evaluated in closed form. What results is

$$G_p(x,y) = \frac{(-1)^{p-1}}{(2p-1)!} \sum_{\ell=0}^{p-1} (-1)^\ell \binom{2p-1}{\ell} \big(y(1-x)\big)^\ell \big(x(1-y)\big)^{2p-\ell-1} \tag{9}$$

for $0 \le x \le y \le 1$. For example,

$$G_3(x,y) = \frac{1}{120} x^3(1-y)^3 \Big(x^2(1-y)^2 - 5xy(1-x)(1-y) + 10y^2(1-x)^2\Big)$$

for these x, y. Figure 3 shows pseudocolor plots of $G_2(x,y)$ and $G_3(x,y)$. Recall that the right picture of Fig. 1 is a pseudocolor plot of $G_1(x,y)$.

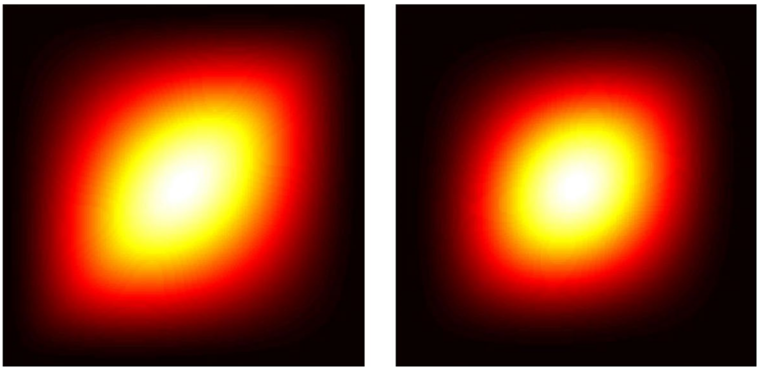

Fig. 3 Pseudocolor plots of $G_2(x,y)$ (left) and $G_3(x,y)$ (right)

However, notice that pseudocolor plots may be misleading. It is right that $G_p(x,y)$ becomes more and more "circular" and concentrated in the center of the square $[0,1]^2$ as p increases, but at the same time the function flattens dramatically: we have

$$G_p(x,x) = \frac{x^{2p-1}(1-x)^{2p-1}}{(2p-1)[(p-1)!]^2},$$

the maximum of which is $1/(4^{2p-1}(2p-1)[(p-1)!]^2)$.

The limiting distribution of the first and last columns and of the trace and the sum of all entries of $T_n^{-1}(\omega_p)$ was also computed in [1, 14, 15].

Theorem 4 *For each fixed* j,

$$_{[nx],j} = [T_n^{-1}(\omega_p)]_{n-[nx],n-j} = \binom{p+j}{j}\frac{x^{p-1}(1-x)^{p-1}}{(p-1)!}n^{p-1} + O(n^{p-2})$$

uniformly in $x \in [0,1]$. *We also have*

$$\operatorname{tr} T_n^{-1}(\omega_p) = \frac{(2p-1)!(2p-2)!}{(4p-1)![(p-1)!]^2}n^{2p} + o(n^{2p}),$$

$$\sum_{j,k=0}^{n-1}[T_n^{-1}(\omega_p)]_{j,k} = \frac{1}{2p+1}\left[\frac{p!}{(2p)!}\right]^2 n^{2p+1} + o(n^{2p+1}).$$

The last two formulas remain true for $T_n^{-1}(a)$ with $a(t) = \omega_p(t)b(t)$ when including the factor $1/b(1)$ into the right-hand sides. With a little more tricky additional factor on the right, the formula for $[T_n^{-1}(\omega_p)]_{[nx],j}$ can also be carried over to $[T_n^{-1}(a)]_{[nx],j}$.

Above we already mentioned Green's function. The connection is as follows. Consider the boundary value problem

$$(-1)^p u^{2p} = v \quad \text{on} \quad [0,1] \tag{10}$$

$$u^{(0)}(0) = \cdots = u^{(p-1)}(0) = 0, \quad u^{(0)}(1) = \ldots = u^{(p-1)}(1) = 0. \tag{11}$$

The Green function for this problem is the function G on $[0,1]^2$ which gives the solution to this boundary value problem by the formula $u(x) = \int_0^1 G(x,y)v(y)\,dy$. Discretization of problem (10), (11) leads to the Toeplitz matrices $T_n(\omega_p)$, and it is therefore not too much a surprise that the Green function for the problem is connected with the inverse $T_n^{-1}(\omega_p)$. This was rigorously proved in [6] for $p = 1$ and by Parter [12] and Widom [23] for general p. In the latter two papers, the authors relate the minimal eigenvalues of truncated discrete and continuous convolutions to the reciprocals of the maximal eigenvalues of an integral operator with some (quite complicated) kernel $K(x, y)$ which is identified as Green's function of problem (10), (11). However, the relation between the entries of $T_n^{-1}(\omega_p b)$ and Green's kernel lies deeper than the relation between the eigenvalues of these two and was uncovered only by Rambour and Seghier [14, 15]. Anyway, eventually we know that $G(x,y) = K(x,y) = G_p(x,y)$. A direct proof (avoiding the detour through Toeplitz matrices) that Green's function is given by (9) can be found in [1]. Paper [5] contains more pieces of information about this and related topics.

Declarations

Conflict of interest The author states that there is no conflict of interest. No datasets were generated or analysed during the current study.

References

1. Böttcher, A.: The constants in the asymptotic formulas by Rambour and Seghier for inverses of Toeplitz matrices. Integral Equ. Oper. Theory **50**, 43–55 (2004)
2. Böttcher, A.: The Duduchava-Roch formula. Oper. Theory: Adv. Appl. **258**, 1–19 (2017)
3. Böttcher, A., Fukshansky, L., Garcia, S.R., Maharaj, H.: Toeplitz determinants with perturbations in the corners. J. Funct. Anal. **268**, 171–193 (2015)
4. Böttcher,A., Silbermann,B.: Introduction to large truncated Toeplitz matrices. Universitext, Springer-Verlag, New York (1999)
5. Böttcher, A., Widom, H.: From Toeplitz eigenvalues through Green's kernels to higher-order Wirtinger–Sobolev inequalities. Oper. Theor: Adv. Appl. **171**, 73–87 (2006)
6. Courant, R., Friedrichs, K., Lewy, H.: Über die partiellen Differenzengleichungen der mathematischen Physik. Math. Ann. **100**, 32–74 (1928)
7. Deift, P., Its, A., Krasovsky, I.: Toeplitz matrices and Toeplitz determinants under the impetus of the Ising model: some history and some recent results. Comm. Pure Appl. Math. **66**, 1360–1438 (2013)
8. Duduchava, R.V.: On discrete Wiener–Hopf equations. Trudy Tbilis. Matem. Inst. **50**, 42–59 (1975). **[in Russian]**
9. Gohberg, I., Feldman, I. A.: Convolution equations and projection methods for their solution. Am. Math. Soc. Providence, RI, 1974 [Russian original: Nauka, Moscow, 1971]
10. Gohberg, I., Sementsul, A.A.: The inversion of finite Toeplitz matrices and their continual analogues. Matem. Issled. **7**, 201–223 (1972). **[in Russian]**
11. Heinig, G., Rost, K.: Algebraic methods for Toeplitz-like matrices and operators. Birkhäuser Verlag, Basel, 1984
12. Parter, S.V.: On the extreme eigenvalues of truncated Toeplitz matrices. Bull. Am. Math. Soc. **67**, 191–196 (1961)
13. Rambour, P., Rinkel, J.-M., Seghier, A.: Inverse asymptotique de la matrice de Toeplitz et noyau de Green. C. R. Acad. Sci. Paris **331**, 857–860 (2000)
14. Rambour, P., Seghier, A.: Exact and asymptotic inverse of the Toeplitz matrix with polynomial singular symbol. C. R. Acad. Sci. Paris **335**, 705–710 (2002). Erratum in C. R. Acad. Sci. Paris, 336 (2003), 399–400
15. Rambour, P., Seghier, A.: Formulas for the inverses of Toeplitz matrices with polynomially singular symbols. Integral Equ. Oper. Theory **50**, 83–114 (2004)
16. Rambour, P., Seghier, A.: Inverse asymptotique des matrices de Toeplitz de symbole $(1-\cos\theta)^\alpha f_1, -1/2 < \alpha \leq 1/2$, et noyaux intégraux. Bull. Sci. Math. **134**, 155–188 (2010)
17. Roch, S.: Das Reduktionsverfahren für Produktsummen von Toeplitzoperatoren mit stückweise stetigen Symbolen. Wiss. Z. Tech. Hochsch. Karl-Marx-Stadt **26**, 265–273 (1984)

18. Simon, B.: Orthogonal polynomials on the unit circle, Part 1: Classical theory. Am. Math. Soc. Colloq. Publ., Vol. 54, Amer. Math. Soc, Providence, RI (2005)
19. Spitzer, F.L., Stone, C.J.: A class of Toeplitz forms and their application to probability theory. Illinois J. Math. **4**, 253–277 (1960)
20. Szegő, G.: Beiträge zur Theorie der Toeplitzschen Formen, Parts I and II. *Math. Z.* **6**, 167–202 (1920); **9**, 167–190 (1921)
21. Szegő, G.: Orthogonal polynomials. Am. Math. Soc. Colloq. Publ., Vol. 23, Amer. Math. Soc, Providence, RI (1939)
22. Trench, W.F.: An algorithm for the inversion of finite Toeplitz matrices. J. Soc. Indust. Appl. Math. **12**, 515–522 (1964)
23. Widom, H.: Extreme eigenvalues of translation kernels. Trans. Am. Math. Soc. **100**, 252–262 (1961)
24. Widom, H.: Asymptotic behavior of block Toeplitz matrices and determinants, II. Adv. Math. **21**, 1–29 (1976)