Numer. Math. (2005) 100: 457–482
Digital Object Identifier (DOI) 10.1007/s00211-005-0596-3

Numerische Mathematik

Explicit inverse of a tridiagonal $k-$Toeplitz matrix*

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Received July 12, 2004 / Revised version received December 31, 2004
Published online: March 30, 2005 –

Dedicated to Professor José Vitória on the occasion of his 65th birthday

Summary. We obtain explicit formulas for the entries of the inverse of a nonsingular and irreducible tridiagonal $k-$Toeplitz matrix A. The proof is based on results from the theory of orthogonal polynomials and it is shown that the entries of the inverse of such a matrix are given in terms of Chebyshev polynomials of the second kind. We also compute the characteristic polynomial of A which enables us to state some conditions for the existence of A^{-1}. Our results also extend known results for the case when the residue $\bmod k$ of the order of A is equal to 0 or $k-1$ (*Numer. Math.*, 10 (1967), pp. 153–161.).

Mathematics Subject Classification (2000): 15A09, 42C05, 33C45, 65Q05

1 Introduction

Tridiagonal matrices arise in many contexts in pure and applied mathematics. For instance, besides their own interest in *linear algebra*, they are a basic tool in *approximation theory*, particularly in the study of *special functions* and *orthogonal polynomials*. They also come out naturally in *numerical analysis* and *partial differential equations*, in the discretization of elliptic or parabolic partial differential equations by finite difference methods. In the application of such methods, the study of the inverse of the involved matrices appears to be very important. For a review of the inverse of a tridiagonal (and block tridiagonal) matrix, as well as applications of tridiagonal and inverse of tridiagonal matrices, we suggest to the reader the paper by G. Meurant [22] as well

* The work was supported by *CMUC* (Centro de Matemática da Universidade de Coimbra) and by *Acção Integrada Luso-Espanhola E-6/03*
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as the references therein. According to [22], D. Moskovitz [23] in 1944 was the first to give an explicit formula for the inverse of a tridiagonal matrix (in connection with one dimensional and two dimensional Poisson problems). A closed explicit formula for the inverse is known from several references in the case of a tridiagonal Toeplitz matrix (cf. P. Schlegel [25], T. Yamamoto and Y. Ikebe [28], Heinig and Rost [11, p.28], R. K. Mallik [18]), i.e., a tridiagonal matrix with constant entries along the diagonals parallel to the main diagonal, which is a matrix that corresponds to a discretization of an elliptic partial differential equation with constant coefficients (cf. (4.26) bellow). In [6] the authors also gave closed explicit formulas for the inverse of an irreducible tridiagonal matrix with 2−periodic and 3−periodic entries along the diagonals parallel to the main diagonals. Other explicit examples for the entries of the inverse of some tridiagonal matrices can be found in Lewis [13]. Formulas (usually not explicit) for the inverse of a general tridiagonal matrix, as well as criteria for a given matrix to have a tridiagonal inverse, also have been given by several authors, some of them involving recurrence relations or some canonical decompositions for the matrices in consideration (for details, see again [22] and the references therein, e.g.). Finally, explicit formulae for the entries of the inverse of a general tridiagonal matrix were given by R. K. Mallik [18] by using an approach based on linear difference equations.

In this paper we generalize the above mentioned formula for the inverse of a tridiagonal Toeplitz and tridiagonal 2−periodic and 3−periodic matrices to some more general matrices. In fact, the purpose of this paper is to calculate explicitly the elements of the inverse of a tridiagonal $k-$Toeplitz matrix, a concept introduced by M. J. C. Gover and S. Barnett [10]. By definition, given a matrix $A = [a_{ij}]$ of order N and a positive integer number $k \leq N$, a tridiagonal matrix A is $k-$Toeplitz if

$$a_{i+k,j+k} = a_{ij} \quad (i, j = 1, 2, \cdots, N-k)\,.$$

This means that A is a tridiagonal matrix of the form

$$A = \begin{pmatrix} a_1 & b_1 & & & & & & & & & \\ c_1 & \ddots & \ddots & & & & & & & & \\ & \ddots & a_k & b_k & & & & & & & \\ & & c_k & a_1 & b_1 & & & & & & \\ & & & c_1 & \ddots & \ddots & & & & & \\ & & & & \ddots & a_k & b_k & & & & \\ & & & & & c_k & a_1 & b_1 & & & \\ & & & & & & c_1 & \ddots & \ddots & & \\ & & & & & & & \ddots & & & \end{pmatrix} \in \mathbb{C}^{N\times N}\,. \tag{1.1}$$

Notice that if $k = 1$ then A is a (tridiagonal) Toeplitz matrix; and when the order N is a multiple of k then A is a block Toeplitz matrix. If $b_i c_i \neq 0$ for all $i = 1, \cdots, k$ we say that A is irreducible. In this paper we will assume that A is irreducible.

The structure of the paper is as follows. In the next section some basic tools concerning the general theory of orthogonal polynomials are presented. We also consider systems of orthogonal polynomials that can be obtained from other ("old") ones via a polynomial mapping, in some appropriate way describe further on, and we obtain explicit formulas, in terms of the "old" polynomials, for the ("new") polynomials obtained by the polynomial mapping. In section 3 a review of some known facts concerning the inverse of a tridiagonal matrix is given, pointing out the connection with the theory of orthogonal polynomials. An application of the results in the previous sections is given in section 4, where we give explicit expressions for the entries of the inverse of the tridiagonal $k-$Toeplitz matrix A. Essentially we show that the entries of this inverse can be computed by using an appropriate polynomial mapping taking as "old" polynomials the classical Chebyshev polynomials of the second kind. Our results are special cases of the general formulas given in [18], but we would like to point out that our approach gives more concise formulas, taking into account the special structure of the matrices treated here. On the other hand, the conjugation of our results together with the ones in [18] will lead to some interesting formulas giving closed expressions, in terms of Chebyshev polynomials, for certain intricate sums. The results presented in section 4 are stated assuming that the matrix A is nonsingular and so in section 5 we state conditions for the existence of A^{-1}. These conditions will be obtained from an explicit expression for the characteristic polynomial of A. Such expression generalizes results by L. Elsner and R. M. Redheffer [5] stated for the case when the residue (mod k) of the order of A equals 0 or $k - 1$.

2 Preliminary results on orthogonal polynomials

Most of the basic facts from the general theory of orthogonal polynomials presented in this section can be founded in the books by G. Szegö [26] and T. S. Chihara [4]. The theoretical basis for most orthogonality proofs in this paper is the Favard's theorem (also called the spectral theorem for orthogonal polynomials), which states that any orthogonal polynomial sequence (OPS) $\{P_n\}_{n\geq 0}$ is characterized by a three-term recurrence relation

$$x P_n(x) = \alpha_n P_{n+1}(x) + \beta_n P_n(x) + \gamma_n P_{n-1}(x) , \quad n = 0, 1, 2, \cdots \tag{2.2}$$

with initial conditions $P_{-1}(x) = 0$ and $P_0(x) = \text{const.} \neq 0$, where $\{\alpha_n\}_{n\geq 0}$, $\{\beta_n\}_{n\geq 0}$ and $\{\gamma_n\}_{n\geq 0}$ are sequences of complex numbers such that $\alpha_n \gamma_{n+1} \neq 0$

for all $n = 0, 1, 2, \cdots$. If $\alpha_n = 1$ for all $n = 0, 1, 2, \cdots$ then each P_n is a monic orthogonal polynomial of degree exactly n, and we say that $\{P_n\}_{n\geq 0}$ is a monic orthogonal polynomial sequence (MOPS).

In matrix form the three-term recurrence relation (2.2) can be written as

$$x\begin{pmatrix} P_0(x) \\ P_1(x) \\ \vdots \\ P_n(x) \end{pmatrix} = J_{n+1}\begin{pmatrix} P_0(x) \\ P_1(x) \\ \vdots \\ P_n(x) \end{pmatrix} + \alpha_n P_{n+1}(x)\begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix},$$

where J_{n+1} is a tridiagonal Jacobi matrix of order $n+1$, defined by

$$J_{n+1} := \begin{pmatrix} \beta_0 & \alpha_0 & 0 & \cdots & 0 & 0 \\ \gamma_1 & \beta_1 & \alpha_1 & \cdots & 0 & 0 \\ 0 & \gamma_2 & \beta_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \beta_{n-1} & \alpha_{n-1} \\ 0 & 0 & 0 & \cdots & \gamma_n & \beta_n \end{pmatrix} \quad (n = 0, 1, 2, \cdots).$$

(In fact, usually a Jacobi matrix is understanded as a real symmetric tridiagonal matrix, but here we avoid this distinction.) Hence if $\{x_{nj}\}_{j=1}^n$ is the set of zeros of the polynomial P_n then each x_{nj} is an eigenvalue of the corresponding Jacobi matrix J_n of order n, and an associated eigenvector is $[\, P_0(x_{nj}), P_1(x_{nj}), \cdots, P_{n-1}(x_{nj})\,]^t$. Moreover, the (monic) characteristic polynomial of J_n is precisely P_n, i.e.,

$$P_n(x) = \det\,(xI_n - J_n)\;, \quad n = 1, 2, \cdots,$$

where I_n denotes the identity matrix of order n.

Two of the most useful OPS's are the Chebyshev polynomials of the first and second kind, denoted by $\{T_n\}_{n\geq 0}$ and $\{U_n\}_{n\geq 0}$, respectively. These polynomials satisfy the three-term recurrence relations

$$\begin{aligned} 2xT_n(x) &= T_{n+1}(x) + T_{n-1}(x)\,, \quad T_0(x) = 1\,, \quad T_1(x) = x\,, \\ 2xU_n(x) &= U_{n+1}(x) + U_{n-1}(x)\,, \quad U_0(x) = 1\,, \quad U_1(x) = 2x\,, \end{aligned} \tag{2.3}$$

for all $n = 1, 2, \cdots$. It is well known that U_n and T_n also satisfy

$$T_n(x) = \cos(n\theta)\,, \quad U_n(x) = \frac{\sin(n+1)\theta}{\sin\theta}\,, \quad x = \cos\theta \quad (0 \leq \theta \leq \pi)$$

for all $n = 0, 1, 2 \cdots$ (where, if $\sin\theta = 0$, $\sin(n+1)\theta/\sin\theta$ must be replaced by its limit as $\theta \to 0$), from which one easily deduce the orthogonality relations

$$\int_{-1}^{1} T_n(x)T_m(x)\frac{\mathrm{d}x}{\sqrt{1-x^2}} = \begin{cases} \pi & \text{if } n = m = 0 \\ \frac{\pi}{2}\,\delta_{n,m} & \text{otherwise}\,, \end{cases}$$

and

$$\int_{-1}^{1} U_n(x)U_m(x)\,\sqrt{1-x^2}\,\mathrm{d}x = \tfrac{\pi}{2}\,\delta_{n,m}\,,$$

as well as the explicit formulas

$$T_n(z) = \frac{n}{2}\sum_{\nu=0}^{\lfloor n/2\rfloor}(-1)^{\nu}\frac{(n-\nu-1)!}{\nu!(n-2\nu)!}\,(2z)^{n-2\nu} \quad (n=1,2,\cdots)\,,$$

$$U_n(z) = \sum_{\nu=0}^{\lfloor n/2\rfloor}(-1)^{\nu}\frac{(n-\nu)!}{\nu!(n-2\nu)!}\,(2z)^{n-2\nu} \quad (n=0,1,2,\cdots)\,, \tag{2.4}$$

where $\lfloor x\rfloor$ denotes the greater integer less or equal to the real number x. Further, the asymptotic result

$$\lim_{n\to+\infty}\frac{U_n(z)}{U_{n-1}(z)} = z+\sqrt{z^2-1} \tag{2.5}$$

holds, where this complex square root is taken in such a way that $z+\sqrt{z^2-1}$ is an analytic function in $\mathbb{C}\setminus[-1,1]$ with $|z+\sqrt{z^2-1}\,| > 1$ when $z\notin[-1,1]$.

Next we will describe some polynomial transformations on orthogonal polynomials which will be used to study $k-$Toeplitz matrices. Let $\{p_n(x)\}_{n\geq 0}$ be any MOPS. According to the Favard theorem it can be characterized by a three-term recurrence relation. For our purposes, it is convenient to write this recurrence as a general block of recurrence relations of the type

$$\begin{aligned}(x-b_n^{(j)})p_{nk+j}(x) &= p_{nk+j+1}(x)+a_n^{(j)}\,p_{nk+j-1}(x)\,,\\ &\qquad j=0,1,\cdots,k-1\,;\quad n=0,1,2,\cdots\,,\end{aligned} \tag{2.6}$$

and satisfying initial conditions

$$p_{-1}(x)=0\,,\quad p_0(x)=1\,.$$

Without lost of generality, we will take $a_0^{(0)}=1$, and polynomials p_s with $s\leq -1$ will be always defined as the zero polynomial. Also, we make the convention that empty sum equals zero, and empty product equals one. Since we assume that $\{p_n(x)\}_{n\geq 0}$ given by (2.6) is a sequence of orthogonal polynomials, we need to impose the conditions

$$a_n^{(j)}\neq 0\,,\quad j=0,1,\cdots,k-1\,;\; n=0,1,2,\cdots\,.$$

We also assume that $k \geq 3$. Following J. Charris, M. E. H. Ismail and S. Monsalve [3], for $n = 0, 1, 2, \cdots$, we introduce polynomials $\Delta_n(i, j; \cdot)$ by

$$\Delta_n(i, j; x) := \begin{cases} 0 & \text{if } j < i - 2 \\ 1 & \text{if } j = i - 2 \\ x - b_n^{(i-1)} & \text{if } j = i - 1 \end{cases}$$

and, for $j \geq i \geq 1$, by the determinantal form

$$\Delta_n(i, j; x) := \begin{vmatrix} x - b_n^{(i-1)} & 1 & 0 & \cdots & 0 & 0 \\ a_n^{(i)} & x - b_n^{(i)} & 1 & \cdots & 0 & 0 \\ 0 & a_n^{(i+1)} & x - b_n^{(i+1)} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & x - b_n^{(j-1)} & 1 \\ 0 & 0 & 0 & \cdots & a_n^{(j)} & x - b_n^{(j)} \end{vmatrix} .$$

In [3] the authors showed that in order to determine the polynomials p_n for all $n = 0, 1, 2, \cdots$, it is only need to compute the p_{nk}'s for all $n = 0, 1, 2, \cdots$. A special case of main interest in applications occurs when the given MOPS $\{p_n\}_{n\geq 0}$ is obtained from another MOPS $\{q_n\}_{n\geq 0}$ via a polynomial mapping, in the sense that there exists a polynomial T of degree exactly k such that, up to an affine change in the variables,

$$p_{nk}(x) = q_n(T(x)) , \quad n = 0, 1, 2, \cdots . \tag{2.7}$$

Assurance of the existence of such an orthogonal sequence $\{q_n\}_{n\geq 0}$ is not easy in practice. It is known, e.g., that if $\{p_n\}_{n\geq 0}$ is obtained from some other system of orthogonal polynomials via a polynomial mapping (in the above sense) then $b_n^{(0)}$ and $\Delta_n(2, k-1; x)$ must be independent of n (see [3],[8]). This, however, is not a sufficient condition, as examples show. A sufficient condition has been improved in [3] (cf. Theorem 4.1 and Remark 4.2), and it states that if both $b_n^{(0)}$ and $\Delta_n(2, k-1; x)$ are independent of n and if, in addition,

$$a_n^{(0)} \Delta_{n-1}(2, k-2; x) + a_n^{(1)} \Delta_n(3, k-1; x) - a_0^{(1)} \Delta_0(3, k-1; x)$$

is independent of x for every $n = 1, 2, \cdots$, then $\{p_n\}_{n\geq 0}$ can be obtained via a polynomial mapping of the type (2.7). These kind of polynomial mappings, such as (2.7), were extensively studied by J. Geronimo and W. Van-Assche in [8] and J. Charris and M. E. H. Ismail in [2]. Some examples, making a connection with the so-called sieved orthogonal polynomials on the real line and on the unit circle, were given in [12] and [24]. Other examples and applications, in the particular cases of quadratic and cubic polynomial mappings, appear in [1], [19], [20] and [21].

A polynomial mapping of the type (2.7) comes essentially from the expansion of the p_{nk+j}'s in terms of p_{nk} and $p_{(n+1)k}$. Next we consider a slightly different polynomial mapping, which we found to be more appropriate to study tridiagonal $k-$Toeplitz matrices. The idea consists of expanding the p_{nk+j}'s in terms of p_{nk-1} and $p_{(n+1)k-1}$, which will lead to a polynomial mapping of the type

$$p_{nk+k-1}(x) = \rho(x) q_n(T(x)) \,, \quad n = 0, 1, 2, \cdots ,$$

where ρ and T are fixed polynomials of degree $k-1$ and k, respectively. This fact is stated in the next proposition.

Theorem 2.1 *Let $\{p_n\}_{n\geq 0}$ be a MOPS characterized by the general block of recurrence relations* (2.6). *For $n = 0, 1, 2, \cdots$, define*

$$\begin{aligned} r_n(x) := {} & a^{(0)}_{n+1} \Delta_{n+1}(2, k-2; x) - a^{(0)}_1 \Delta_1(2, k-2; x) \\ & + a^{(k-1)}_n \Delta_n(1, k-3; x) - a^{(k-1)}_0 \Delta_0(1, k-3; x) \,. \end{aligned}$$

Assume that, for all $n = 0, 1, 2, \cdots$, the following conditions hold:

(i) $b^{(k-1)}_n$ *is independent of n ;*
(ii) $\Delta_n(1, k-2; x) =: \rho(x)$ *is independent of n for every x ;*
(iii) $r_n(x) =: r_n$ *is independent of x for every n .*

Consider the polynomial T of degree k defined as

$$T(x) := \Delta_0(1, k-1; x) - a^{(0)}_1 \Delta_1(2, k-2; x) \,,$$

and let $\{q_n\}_{n\geq 0}$ be the MOPS generated by the recurrence relation

$$q_{n+1}(x) = (x - r_n)\, q_n(x) - s_n q_{n-1}(x) \,, \quad n = 0, 1, 2, \cdots \tag{2.8}$$

with initial conditions $q_{-1}(x) = 0$ and $q_0(x) = 1$, where

$$s_n := a^{(0)}_n a^{(1)}_n \cdots a^{(k-1)}_n \,.$$

Then, for each $j = 0, 1, 2, \cdots , k-1$ and all $n = 0, 1, 2, \cdots$,

$$\begin{aligned} p_{kn+j}(x) = {} & \Delta_n(1, j-1; x)\, q_n(T(x)) \\ & + a^{(0)}_n a^{(1)}_n \cdots a^{(j)}_n \Delta_n(j+2, k-2; x)\, q_{n-1}(T(x)) \,. \end{aligned} \tag{2.9}$$

In particular, for $j = k-1$,

$$p_{kn+k-1}(x) = \rho(x)\, q_n(T(x)) \,, \quad n = 0, 1, 2, \cdots \,. \tag{2.10}$$

Proof The proof is based on the approach developed in [2] and [3]. We begin by rewriting (2.6) as a system in matrix form,

$$V\begin{pmatrix} p_{nk} \\ p_{nk+1} \\ \vdots \\ p_{nk+k-3} \\ p_{nk+k-2} \\ p_{(n+1)k} \end{pmatrix} = \begin{pmatrix} a_n^{(0)} p_{nk-1} \\ 0 \\ \vdots \\ 0 \\ p_{(n+1)k-1} \\ (x-b_n^{(k-1)}) p_{(n+1)k-1} \end{pmatrix},$$

where V is the tridiagonal matrix of order k defined by

$$V := \begin{pmatrix} x-b_n^{(0)} & -1 & & & & & \\ -a_n^{(1)} & x-b_n^{(1)} & -1 & & & & \\ & -a_n^{(2)} & x-b_n^{(2)} & -1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -a_n^{(k-3)} & x-b_n^{(k-3)} & -1 & \\ & & & & -a_n^{(k-2)} & x-b_n^{(k-2)} & 0 \\ & & & & & a_n^{(k-1)} & 1 \end{pmatrix}.$$

Solving this system for p_{nk+j} in terms of p_{nk+k-1} and p_{nk-1} by Cramer's rule, it follows that the polynomials of the sequence $\{p_n\}_{n\geq 0}$ satisfy the relations

$$\begin{aligned} \Delta_n(1,k-2;x)p_{nk+j}(x) &= \Delta_n(1,j-1;x)p_{(n+1)k-1}(x) \\ &+a_n^{(0)}a_n^{(1)}\cdots a_n^{(j)}\Delta_n(j+2,k-2;x)p_{nk-1}(x)\,, \\ & j=0,1,\cdots,k-2\,,\quad n=0,1,2,\cdots \end{aligned} \tag{2.11}$$

and

$$\begin{aligned} &\Delta_n(1,k-2;x)p_{nk+k}(x) \\ &\quad= \left\{(x-b_n^{(k-1)})\Delta_n(1,k-2;x)-a_n^{(k-1)}\Delta_n(1,k-3;x)\right\}p_{(n+1)k-1}(x) \\ &\qquad -a_n^{(0)}a_n^{(1)}\cdots a_n^{(k-1)}p_{nk-1}(x)\,, \qquad\qquad n=0,1,2,\cdots\,. \end{aligned} \tag{2.12}$$

Hence, one sees that in order to determine the polynomials p_i for all $i = 0,1,2,\cdots$, we only need to compute the p_{nk-1}'s for all $n=0,1,2,\cdots$. In (2.11) replacing n by $n+1$ and then setting $j=0$ we get

$$\begin{aligned} &\Delta_{n+1}(1,k-2;x)p_{nk+k}(x) \\ &\quad= p_{(n+2)k-1}(x)+a_{n+1}^{(0)}\Delta_{n+1}(2,k-2;x)p_{(n+1)k-1}(x) \end{aligned} \tag{2.13}$$

for every $n=0,1,2,\cdots$. Since $\Delta_n(1,k-2;x)$ is independent of n, the left-hand sides of (2.12) and (2.13) coincide, so that (after a new change of indices $n \to n-1$),

$$\begin{aligned} & p_{(n+1)k-1}(x) + a_{n-1}^{(0)} a_{n-1}^{(1)} \cdots a_{n-1}^{(k-1)} p_{(n-1)k-1}(x) \\ & \quad = \Big\{ (x - b_0^{(k-1)}) \Delta_0(1, k-2; x) - a_{n-1}^{(k-1)} \Delta_{n-1}(1, k-3; x) \\ & \qquad - a_n^{(0)} \Delta_n(2, k-2; x) \Big\} p_{nk-1}(x) , \quad n = 1, 2, \cdots . \end{aligned} \tag{2.14}$$

Now, expansion of the determinant $\Delta_0(1, k-1; x)$ along its last row gives

$$\Delta_0(1, k-1; x) = (x - b_0^{(k-1)}) \Delta_0(1, k-2; x) - a_0^{(k-1)} \Delta_0(1, k-3; x) .$$

Therefore, (2.14) can be rewritten as

$$\begin{aligned} & p_{(n+1)k-1}(x) + a_{n-1}^{(0)} a_{n-1}^{(1)} \cdots a_{n-1}^{(k-1)} p_{(n-1)k-1}(x) \\ & \quad = \Big\{ \Delta_0(1, k-1; x) + a_0^{(k-1)} \Delta_0(1, k-3; x) \\ & \qquad - a_{n-1}^{(k-1)} \Delta_{n-1}(1, k-3; x) - a_n^{(0)} \Delta_n(2, k-2; x) \Big\} p_{nk-1}(x) \\ & \quad = \{ T(x) - r_{n-1}(x) \} p_{nk-1}(x) \end{aligned}$$

for all $n = 1, 2, \cdots$, hence

$$\begin{aligned} p_{(n+1)k-1}(x) = (T(x) - r_{n-1}) p_{nk-1}(x) - s_{n-1} p_{(n-1)k-1}(x) , \\ n = 1, 2, \cdots . \end{aligned}$$

Since $p_{k-1}(x) = \Delta_0(1, k-2; x) \equiv \rho(x)$, (2.10) comes now easily by induction over n. Finally, (2.9) is an immediate consequence of (2.11) and (2.10). □

3 Inverse of a tridiagonal matrix

Let us consider a general tridiagonal matrix of order N, say

$$J = \begin{pmatrix} \beta_1 & \alpha_1 & 0 & \cdots & 0 & 0 \\ \gamma_1 & \beta_2 & \alpha_2 & \cdots & 0 & 0 \\ 0 & \gamma_2 & \beta_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \beta_{N-1} & \alpha_{N-1} \\ 0 & 0 & 0 & \cdots & \gamma_{N-1} & \beta_N \end{pmatrix} . \tag{3.15}$$

When J is invertible, J^{-1} can be computed according to the following result.

Proposition 3.1 (Usmani [27]) *Assume that J is nonsingular. Then the entries of J^{-1} are given by*

$$(J^{-1})_{ij} = \begin{cases} (-1)^{i+j} \alpha_i \cdots \alpha_{j-1} \theta_{i-1} \phi_{j+1} / \theta_N & \text{if } i \le j \\ (-1)^{i+j} \gamma_j \cdots \gamma_{i-1} \theta_{j-1} \phi_{i+1} / \theta_N & \text{if } i > j , \end{cases} \tag{3.16}$$

where $\theta_{-1}=0\,,\ \theta_0=1\,,$

$$\theta_n=\beta_n\theta_{n-1}-\alpha_{n-1}\gamma_{n-1}\theta_{n-2}\quad(n=1,2,\cdots,N)\,, \tag{3.17}$$

and $\phi_{N+2}=0\,,\ \phi_{N+1}=1\,,$

$$\phi_n=\beta_n\phi_{n+1}-\alpha_n\gamma_n\phi_{n+2}\quad(n=N,N-1,\cdots,1)\,. \tag{3.18}$$

Henceforth, one sees that the problem of the determination of the inverse of a (nonsingular) tridiagonal matrix reduces to solving the difference equations (3.17) and (3.18). Those are homogeneous linear difference equations of second order with variable coefficients. The explicit solutions to such difference equations (in the general case, with variable coefficients) were found in the last years by R. K. Mallik (see [14]–[18]). In fact, based on these results on difference equations, in [18] explicit formulas for the entries of the inverse of a general tridiagonal matrix were given, only in terms of the entries of the matrix. These results can be summarized in the following proposition, where the definition of a set $S_q(m+1,n)$ is needed, which has been introduced in [14] as follows: for $q,L,U\in\mathbb{N}$, $S_q(L,U)$ is the set of all $q-$tuples with elements from $\{L,L+1,\cdots,U\}$ arranged in ascending order so that no two consecutive elements are present, i.e.,

$$S_q(L,U):=\begin{cases}\{L,L+1,\cdots,U\}\,, & \text{if } U\ge L \text{ and } q=1\ ;\\ \Big\{(k_1,\cdots,k_q)\ :\ k_1,\cdots,k_q\in\{L,L+1,\cdots,U\} \text{ and} & \\ \qquad\qquad k_\ell-k_{\ell-1}\ge 2 \text{ for } \ell=2,\cdots,q\Big\}\,, & \\ \qquad \text{if } U\ge L+2 \text{ and } 2\le q\le\lfloor (U-L+2)/2\rfloor\ ; & \\ \emptyset\,, & \text{otherwise}\,.\end{cases}$$

Proposition 3.2 (Mallik [18]) *Assume that* J *is irreducible and set*

$$E_n(m):=\begin{cases}(-1)^{n-m+1}\dfrac{1}{\alpha_m\cdots\alpha_n} & \\ \quad\times\left(\beta_m\cdots\beta_n+\displaystyle\sum_{q=1}^{\lfloor (n-m+1)/2\rfloor}\ \sum_{(k_1,\cdots,k_q)\in S_q(m+1,n)}\sigma_{m,n}(k_1,\cdots,k_q)\right)\,, & \\ \qquad \text{if } m=1,\cdots,n-1\ ,\ n=2,\cdots,N\ ; & \\ -\dfrac{\beta_n}{\alpha_n}\,, & \text{if } m=n\ ,\ n=1,\cdots,N\ ;\\ 1\,, & \text{if } m=n+1\ ,\ n=0,\cdots,N\ ;\\ 0\,, & \text{otherwise}\,,\end{cases}$$

where

$$\sigma_{m,n}(k_1,\cdots,k_q):=\beta_m\cdots\beta_n\,(-1)^q\prod_{s=1}^{q}\frac{\alpha_{k_s-1}\gamma_{k_s-1}}{\beta_{k_s-1}\beta_{k_s}}\,.$$

Then J is invertible if and only if $E_N(1) \neq 0$. Under such conditions, the entries of J^{-1} are explicitly given by

$$(J^{-1})_{ij} = \begin{cases} -\dfrac{E_{i-1}(1)E_N(j+1)}{\alpha_j\, E_N(1)} & \text{if } i \leq j \\ -\dfrac{F_{j-1}(1)F_N(i+1)}{\gamma_i\, F_N(1)} & \text{if } i > j\ , \end{cases} \tag{3.19}$$

where, for $m \leq n$,

$$F_n(m) := \frac{\alpha_m \cdots \alpha_n}{\gamma_m \cdots \gamma_n}\, E_n(m)\ .$$

Remark The expression for $\sigma_{m,n}(k_1, \cdots, k_q)$ is well defined even if some of the β's are zero, since all the denominators $\beta_{k_s-1}\beta_{k_s}$ $(s = 1, \cdots, q)$ cancel out with some factors in $\beta_m \cdots \beta_n$.

Formulas (3.19) follow from (71)–(72) in [18], and the invertibility condition is a consequence of (77) in [18], which reads as

$$\det J = (-1)^N \alpha_1 \cdots \alpha_N\, E_N(1)\ . \tag{3.20}$$

Further, it follows from (18) and (63a)–(63b) in [18] that $E_n(m)$ satisfies

$$E_n(m) = -\frac{\beta_n}{\alpha_n}\, E_{n-1}(m) - \frac{\gamma_{n-1}}{\alpha_n}\, E_{n-2}(m)\ , \quad 1 \leq n \leq N\ , \ \ 1 \leq m \leq n. \tag{3.21}$$

This recurrences, together with the relations

$$\begin{gathered} E_{-1}(1) = 0\ , \quad E_n(n+1) = 1 \quad (0 \leq n \leq N)\ , \\ E_n(n) = -\frac{\beta_n}{\alpha_n} \quad (1 \leq n \leq N)\ , \end{gathered} \tag{3.22}$$

can be used to determine all the $E_n(m)$ for $1 \leq n \leq N$ and $1 \leq m \leq n$. In fact, Mallik found the explicit expressions (3.19) for the entries of J^{-1} by solving recurrences (3.21)–(3.22), as well as

$$E_n(m) = -\frac{\beta_m}{\alpha_m}\, E_n(m+1) - \frac{\gamma_m}{\alpha_{m+1}}\, E_n(m+2), \ \ 1 \leq m \leq n\ , \ 1 \leq n \leq N \tag{3.23}$$

(cf. (25) and (63a)–(63b) in [18]). Now, using (3.17) and (3.21)–(3.22) one sees that

$$\theta_n = (-1)^n\, \alpha_1 \cdots \alpha_n\, E_n(1)\ , \quad -1 \leq n \leq N\ . \tag{3.24}$$

Similarly, using (3.18) and (3.22)–(3.23) one verifies that

$$\phi_n = (-1)^{N-n+1}\, \alpha_n \cdots \alpha_N\, E_N(n)\ , \quad 1 \leq n \leq N+2\ . \tag{3.25}$$

These relations (3.24)–(3.25) show that Propositions 3.1 and 3.2 are consistent. In fact, Proposition 3.1 can now be derived from Proposition 3.2.

Notice that the above difference equations (3.17)–(3.18), or (3.21)–(3.23), also make clear a connection between the theory of orthogonal polynomials and the problem of the inversion of a tridiagonal matrix. This connection has been explored by the authors in [6] to evaluate the inverse of tridiagonal $2-$Toeplitz and $3-$Toeplitz matrices. We point out that the technique used in [6] is not easy to apply to the general case of the tridiagonal $k-$Toeplitz matrix, since it does not give a general procedure to solve the mentioned difference equations. On the other hand, in practice (depending on the specific structure of the given matrix J) it may be hard to work with the explicit expression for $E_n(m)$ as in Proposition 3.2. In the next section it will be shown, using the results presented in section 2, that the difference equations (3.17)–(3.18), or (3.21)–(3.23), can be solved for the case of the tridiagonal $k-$Toeplitz matrices in terms of the Chebyshev polynomials of the second kind and an appropriate polynomial mapping. As an indirect consequence, the conjugation of our results together with the ones in Proposition 3.2 will lead to some interesting closed formulas, in terms of Chebyshev polynomials, for some sums involving the sets $S_q(U, L)$.

4 Inverse of a tridiagonal $k-$Toeplitz matrix

Explicit formulas for the inverse of a nonsingular tridiagonal $k-$Toeplitz matrix A such as (1.1) have been given in the case $k = 1$ by several authors (see some references in the introduction). In this case A reduces to a tridiagonal Toeplitz matrix, say

$$\begin{pmatrix} a & b & & & \\ c & a & b & & \\ & c & a & \ddots & \\ & & \ddots & \ddots & b \\ & & & c & a \end{pmatrix},$$

and so, if A is nonsingular and irreducible, putting $d := a/(2\sqrt{bc})$, the inverse is given by

$$(A^{-1})_{ij} = \begin{cases} (-1)^{i+j} \dfrac{b^{j-i}}{\left(\sqrt{bc}\right)^{j-i+1}} \dfrac{U_{i-1}(d)\, U_{n-j}(d)}{U_n(d)} & \text{if } i \le j \\[2ex] (-1)^{i+j} \dfrac{c^{i-j}}{\left(\sqrt{bc}\right)^{i-j+1}} \dfrac{U_{j-1}(d)\, U_{n-i}(d)}{U_n(d)} & \text{if } i > j\,. \end{cases} \tag{4.26}$$

When $k = 2$ the inverse of the (assumed irreducible and nonsingular) tridiagonal $2-$Toeplitz matrix (1.1) has been given in [6]: if we put

$$\mu^2 := b_1 b_2 c_1 c_2 \,, \quad \beta^2 := b_2 c_2 / b_1 c_1 \,,$$
$$\xi_2(x) := \frac{1}{2\mu} \, \{(x - a_1)(x - a_2) - b_1 c_1 - b_2 c_2\}$$

and define $\{Q_i(\cdot; \alpha, \gamma)\}_{i \geq 0}$ the sequence of monic polynomials such that

$$Q_{2i+1}(x; \alpha, \gamma) := (x - \alpha)\, \mu^i \, U_i \, (\xi_2(x)) \,,$$
$$Q_{2i}(x; \alpha, \gamma) := \mu^i \, \{U_i \, (\xi_2(x)) + \gamma \, U_{i-1} \, (\xi_2(x))\} \,,$$

where α and γ are some parameters, then

$$(A^{-1})_{ij} = \begin{cases} (-1)^{i+j} \, b_{p_i}^{\lfloor (j-i)/2 \rfloor} \, b_{q_i}^{\lfloor (j-i+1)/2 \rfloor} \, \theta_{i-1} \, \phi_{j+1} / \theta_n \,, & \text{if } i \leq j \\ (-1)^{i+j} \, c_{p_j}^{\lfloor (j-i)/2 \rfloor} \, c_{q_j}^{\lfloor (j-i+1)/2 \rfloor} \, \theta_{j-1} \, \phi_{i+1} / \theta_n \,, & \text{if } i > j \end{cases} \tag{4.27}$$

where $p_\ell = (3 - (-1)^\ell)/2 \,,\; q_\ell = (3 + (-1)^\ell)/2 \,,$

$$\theta_i = (-1)^i \, Q_i \, (0; a_1, \beta) \,,$$

and

$$\phi_i = \begin{cases} (-1)^i \, Q_{n+1-i} \, (0; a_1, 1/\beta) & \text{if } n \text{ is odd} \\ (-1)^{i+1} Q_{n+1-i} \, (0; a_2, \beta) & \text{if } n \text{ is even} . \end{cases}$$

Notice that (4.26) follows from (4.27) when we take $a_1 = a_2 = a, b_1 = b_2 = b$ and $c_1 = c_2 = c$ (see [6]). The inverse of a tridiagonal nonsingular and irreducible $3-$Toeplitz matrix (case $k = 3$) also have been given in [6], but we point out that a misprint appeared in the statement of the corresponding theorem. Nevertheless, the next procedure is valid for any $k \geq 3$.

In order to give the inverse of the general tridiagonal $k-$Toeplitz matrix (1.1), with $k \geq 3$, we need to introduce some notation. We denote

$$\pi_k \begin{pmatrix} z_1, \cdots, z_k \\ w_1, \cdots, w_k \end{pmatrix} ; x \Bigg)$$

$$:= \begin{vmatrix} x + z_1 & 1 & 0 & \cdots & 0 & 0 & 1 \\ w_1 & x + z_2 & 1 & \cdots & 0 & 0 & 0 \\ 0 & w_2 & x + z_3 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & x + z_{k-2} & 1 & 0 \\ 0 & 0 & 0 & \cdots & w_{k-2} & x + z_{k-1} & 1 \\ w_k & 0 & 0 & \cdots & 0 & w_{k-1} & x + z_k \end{vmatrix} ,$$

and

$$\Delta\left(\begin{matrix} z_1, \cdots, z_s \\ w_1, \cdots, w_{s-1} \end{matrix}; x\right) := \begin{vmatrix} x+z_1 & 1 & 0 & \cdots & 0 & 0 \\ w_1 & x+z_2 & 1 & \cdots & 0 & 0 \\ 0 & w_2 & x+z_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & x+z_{s-1} & 1 \\ 0 & 0 & 0 & \cdots & w_{s-1} & x+z_s \end{vmatrix},$$

so that π_k is a monic polynomial of degree exactly k in x, depending on $2k$ given (complex) parameters, and Δ is a monic polynomial of degree s in x which depends on $2s-1$ given parameters (with the usual conventions $\Delta \equiv 0$ if $s < 0$, $\Delta \equiv 1$ if $s = 0$ and $\Delta \equiv x + z_1$ if $s = 1$). Then, if $w_i \neq 0$ holds for every i, putting

$$w^2 := \prod_{i=1}^{k} w_i \tag{4.28}$$

(i.e., we choose w to be a square root of $\prod_{i=1}^{k} w_i$), we set

$$\begin{aligned} &U_{n,k}\left(\begin{matrix} z_1, \cdots, z_k \\ w_1, \cdots, w_k \end{matrix}; x\right) \\ &\quad := w^n\, U_n\left(\frac{1}{2w}\left\{\pi_k\left(\begin{matrix} z_1, \cdots, z_k \\ w_1, \cdots, w_k \end{matrix}; x\right) + (-1)^k\left(w_k + w^2/w_k\right)\right\}\right) \end{aligned}$$

and notice that $U_{n,k}$ is a monic polynomial of degree nk in x. Finally, define a sequence of monic polynomials $\{Q_i\}_{i\geq 0}$ by

$$\begin{aligned} &Q_{nk+j}\left(\begin{matrix} z_1, \cdots, z_k \\ w_1, \cdots, w_k \end{matrix}; x\right) \\ &\quad := \Delta\left(\begin{matrix} z_1, \cdots, z_j \\ w_1, \cdots, w_{j-1} \end{matrix}; x\right) U_{n,k}\left(\begin{matrix} z_1, \cdots, z_k \\ w_1, \cdots, w_k \end{matrix}; x\right) \\ &\qquad + w_k w_1 \cdots w_j\ \Delta\left(\begin{matrix} z_{j+2}, \cdots, z_{k-1} \\ w_{j+2}, \cdots, w_{k-2} \end{matrix}; x\right) \\ &\qquad \times U_{n-1,k}\left(\begin{matrix} z_1, \cdots, z_k \\ w_1, \cdots, w_k \end{matrix}; x\right), \end{aligned}$$

for $n = 0, 1, 2, \cdots$ and $0 \leq j \leq k-1$, each Q_i being a monic polynomial of degree exactly i (for every i). With these notations we can state our main result.

Theorem 4.1 *Let A be the tridiagonal $k-$Toeplitz matrix of order N defined by* (1.1)*, with $N \geq k \geq 3$. Assume that A is non-singular and irreducible. Then*

$$(A^{-1})_{ij} = \begin{cases} (-1)^{i+j}\, \alpha_i\alpha_{i+1}\cdots\alpha_{j-1}\,\theta_{i-1}\,\phi_{j+1}/\theta_N & \text{if } i \le j \\ (-1)^{i+j}\, \gamma_j\gamma_{j+1}\cdots\gamma_{i-1}\,\theta_{j-1}\,\phi_{i+1}/\theta_N & \text{if } i > j\ , \end{cases}$$

where

$$\alpha_{k\ell+s+1} = b_{s+1}\,, \quad \gamma_{k\ell+s+1} = c_{s+1} \quad \left(s = 0, \cdots, k-1\,;\ \ell = 0, \cdots, \lfloor \tfrac{N-s-1}{k} \rfloor\right)\ ,$$

and the θ_n's and the ϕ_n's are explicitly given by

$$\theta_n = Q_n \left(\begin{matrix} a_1, \cdots, a_k \\ b_1c_1, \cdots, b_kc_k \end{matrix}\ ;\ 0 \right)$$

and, r being an integer number characterized by $0 \le r \le k-1$ and $N \equiv r\ (\mathrm{mod}\, k)$,

$$\phi_n = Q_{N+1-n} \left(\begin{matrix} a_r,\, a_{r-1}, \cdots, a_1,\, a_k,\, a_{k-1}, \cdots, a_{r+1} \\ b_{\sigma(r)}c_{\sigma(r)}, \cdots, b_{\sigma(1)}c_{\sigma(1)},\, b_{\sigma(k)}c_{\sigma(k)}, \cdots, b_{\sigma(r+1)}c_{\sigma(r+1)} \end{matrix}\ ;\ 0 \right)\ ,$$

where σ stands for the following cycle of length k:

$$\sigma := (\, r, r-1, \cdots, 1, k, k-1, \cdots, r+1\,)\ ,$$

with $\sigma := (\, k, k-1, \cdots, 1\,)$ if $r = 0$.

Proof According to the considerations in the previous section, the problem of the determination of the inverse of the general tridiagonal $k-$Toeplitz matrix (1.1) reduces to the determination of the transformations θ_n and ϕ_n from (3.17)–(3.18). In order to evaluate θ_n, notice that for the matrix (1.1) relations (3.17) become the following system of difference equations

$$\theta_{nk+j+1} = a_{j+1}\theta_{nk+j} - b_jc_j\theta_{nk+j-1}\,,$$
$$j = 0, 1, \cdots, k-1\,;\ n = 0, 1, 2, \cdots, \lfloor (N-j-1)/k \rfloor\,,$$

with initial conditions $\theta_{-1} = 0$ and $\theta_0 = 1$. Hence, one sees that

$$\theta_n = p_n(0)\,, \quad n = 0, 1, \cdots, N\,,$$

where $\{p_n\}_{n\ge 0}$ is the MOPS given by the block of recurrence relations (2.6) with $\{a_n^{(j)}\}$ and $\{b_n^{(j)}\}$ defined by

$$a_n^{(0)} = b_kc_k\,, \quad a_n^{(j)} = b_jc_j \quad (j = 1, 2, \cdots, k-1)\,,$$
$$b_n^{(j)} = -a_{j+1} \quad (j = 0, 1, \cdots, k-1)\,. \tag{4.29}$$

Under these conditions, it is clear that all the determinants $\Delta_n(i, j; x)$ are independent of n and $r_n(x) \equiv 0$ is independent of x, so that all the hypothesis (i)–(iii) of Theorem 2.1 are fulfilled. Moreover,

$$r_0 = r_n = 0\,, \quad s_n = \text{const.} = \prod_{i=1}^{k} b_ic_i =: \mu^2\,, \quad n = 1, 2, \cdots,$$

and it follows that in this case the sequence $\{q_n\}_{n\geq 0}$ defined in Theorem 2.1 is explicitly given in terms of the Chebychev polynomials of the second kind by

$$q_n(x) = \mu^n \, U_n\left(\frac{x}{2\mu}\right) \,, \quad n = 0, 1, 2, \cdots$$

(compare with (2.3)). Now, the polynomial T in Theorem 2.1 is given by

$$T(x) = \Delta_0(1, k-1; x) - b_k c_k \Delta_0(2, k-2; x) \,, \tag{4.30}$$

and by some computations on the determinant bellow one easily verifies that

$$\begin{aligned} T(x) + (-1)^{k+1}\left(b_k c_k + \prod_{i=1}^{k-1} b_i c_i\right) \\ &= \begin{vmatrix} x+a_1 & 1 & 0 & \cdots & 0 & 1 \\ b_1 c_1 & x+a_2 & 1 & \cdots & 0 & 0 \\ 0 & b_2 c_2 & x+a_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & x+a_{k-1} & 1 \\ b_k c_k & 0 & 0 & \cdots & b_{k-1}c_{k-1} & x+a_k \end{vmatrix} \\ &= \pi_k\left(\begin{matrix} a_1, \cdots, a_k \\ b_1 c_1, \cdots, b_k c_k \end{matrix} \; ; \; x\right) \end{aligned} \tag{4.31}$$

(notice that the first equality is true since $k \geq 3$). It follows that

$$q_n(T(x)) = U_{n,k}\left(\begin{matrix} a_1, \cdots, a_k \\ b_1 c_1, \cdots, b_k c_k \end{matrix} \; ; \; x\right) \,, \quad n = 0, 1, 2, \cdots .$$

Further, notice that in this case we have

$$\begin{aligned} \Delta_n(1, j-2; x) &= \Delta\left(\begin{matrix} a_1, \cdots, a_j \\ b_1 c_1, \cdots, b_{j-1} c_{j-1} \end{matrix} \; ; \; x\right) \,, \\ \Delta_n(j+2, k-2; x) &= \Delta\left(\begin{matrix} a_{j+2}, \cdots, a_{k-1} \\ b_{j+2} c_{j+2}, \cdots, b_{k-2} c_{k-2} \end{matrix} \; ; \; x\right) . \end{aligned}$$

As a consequence, from (2.9) we conclude that

$$p_n(x) = Q_n\left(\begin{matrix} a_1, \cdots, a_k \\ b_1 c_1, \cdots, b_k c_k \end{matrix} \; ; \; x\right) \,, \quad n = 0, 1, 2, \cdots . \tag{4.32}$$

Hence the representation for θ_n as in the theorem is proved. In order to compute the ϕ_n's, notice first that (3.18) gives

$$\begin{aligned} &\phi_{nk+j} = a_{j+1}\phi_{nk+j+1} - b_j c_j \phi_{nk+j+2} \,, \\ &\qquad j = 0, 1, \cdots, k-1 \, ; \; n = 0, 1, 2, \cdots, \lfloor (N-j)/k \rfloor \,, \end{aligned} \tag{4.33}$$

with initial conditions $\phi_{N+2} = 0$ and $\phi_{N+1} = 1$. To find the solution of (4.33) it is convenient to make a change of variables. Set

$$\psi_n := \phi_{N+1-n}\,, \quad n = 1, 2, \cdots, N\,.$$

Let r be the integer number characterized by

$$0 \le r \le k-1\,, \quad N \equiv r\,(\mathrm{mod}\,k)\,.$$

Then (by straightforward computations) from (4.33) we obtain

$$\psi_{nk+j+1} = b_n^{(j)}\psi_{nk+j} - a_n^{(j)}\psi_{nk+j-1}\,,$$
$$j = 0, 1, \cdots, k-1\,;\ n = 0, 1, 2, \cdots, \lfloor (N-j)/k \rfloor\,,$$

with initial conditions $\psi_{-1} = 0$ and $\psi_0 = 1$, where

$$(4.34) \qquad a_n^{(j)} := \begin{cases} b_{r-j}\,c_{r-j} & \text{if } 0 \le j < r \\ b_{k+r-j}\,c_{k+r-j} & \text{if } r \le j \le k-1\,, \end{cases}$$

and

$$(4.35) \qquad b_n^{(j)} := \begin{cases} -a_{r-j} & \text{if } 0 \le j < r \\ -\,a_{k+r-j} & \text{if } r \le j \le k-1\,. \end{cases}$$

Therefore, we see that

$$\psi_n = p_n(0)\,, \quad n = 0, 1, 2, \cdots, N\,,$$

where, now, $\{p_n\}_{n\ge 0}$ is the MOPS given by the block of recurrence relations (2.6) with $\{a_n^{(j)}\}$ and $\{b_n^{(j)}\}$ defined by (4.34) and (4.35). Hence, if we proceed *mutatis mutandis* exactly as we have done above for the determination of the θ_n's, for this sequence $\{p_n\}_{n\ge 0}$ we find

$$p_n(x) = Q_n\left(\begin{matrix} a_r,\ a_{r-1}, \cdots,\ a_1,\ a_k,\ a_{k-1}, \cdots,\ a_{r+1} \\ b_{\sigma(r)}c_{\sigma(r)}, \cdots, b_{\sigma(1)}c_{\sigma(1)},\ b_{\sigma(k)}c_{\sigma(k)}, \cdots,\ b_{\sigma(r+1)}c_{\sigma(r+1)} \end{matrix}\ ;\ x\right),$$

where $\sigma := (\,r, r-1, \cdots, 1, k, k-1, \cdots, r+1\,)$ is a cycle of length k. For $x = 0$ this gives ψ_n. Hence we get the desired expression for ϕ_n. □

Remark As remarked before, the case $k = 2$ have been solved in [6] by using an appropriate quadratic transformation. However, the inverse of a tridiagonal $2-$Toeplitz matrix also follows from the case $k = 4$ in the result above, when we take $a_3 = a_1$, $a_4 = a_2$, $b_3 = b_1$, $b_4 = b_2$, $c_3 = c_1$ and $c_4 = c_2$. Of course, when all a_i's are equal as well as all the b_i's and all the c_i's, we also get the inverse of a tridiagonal Toeplitz matrix (case $k = 1$).

In order to see an application of Theorem 4.1, we include an example, where we consider that the matrix A in (1.1) has order $N = 19$, with period $k = 5$, and the entries are given by

$$\begin{aligned}
&a_1 = 1\ , \quad a_2 = 2\ , \quad a_3 = 3\ , \quad a_4 = 4\ , \quad a_5 = 5\ , \\
&b_1 = i\ , \quad b_2 = 2\ , \quad b_3 = b_5 = 1\ , \quad b_4 = 1 - i\ , \\
&c_1 = c_5 = 1\ , \quad c_2 = -1\ , \quad c_3 = 2\sqrt{2}\ , \quad c_4 = 2\ .
\end{aligned}$$

Let us compute, e.g., the entries $(A^{-1})_{15,4}$ and $(A^{-1})_{7,7}$. We begin by computing $\det A = \theta_{19}$ (cf. (3.20) and (3.24)). Notice that for the computation of the $U_{n,k}$'s we need to fix ω from (4.28). Since $\omega^2 = \prod_{j=1}^{5} b_j c_j = -8\sqrt{2}\,(1+i)$, we choose

$$\omega := -2\sqrt{2-\sqrt{2}} + 2\,i\sqrt{2+\sqrt{2}}\ .$$

Therefore, by Theorem 4.1 we have

$$\begin{aligned}
\det A = \theta_{19} &= Q_{3\times 5+4}\left(\begin{matrix} 1, 2, 3, 4, 5 \\ i, -2, 2\sqrt{2}, 2-2i, 1 \end{matrix}\ ;\ 0\right) \\
&= \Delta\left(\begin{matrix} 1, 2, 3, 4 \\ i, -2, 2\sqrt{2}, 2-2i \end{matrix}\ ;\ 0\right) U_{3,5}\left(\begin{matrix} 1, 2, 3, 4, 5 \\ i, -2, 2\sqrt{2}, 2-2i, 1 \end{matrix}\ ;\ 0\right) \\
&= (15185728 - 1685504\sqrt{2}) - i\,(79315648 - 39653440\sqrt{2})\ .
\end{aligned}$$

The last equality is easily derived using MATHEMATHICA, e.g.—in this program the Chebyshev polynomials of the second kind are already pre-defined. To compute $(A^{-1})_{15,4}$ we must determine θ_3 and ϕ_{16} in Theorem 4.1. We have

$$\theta_3 = Q_{0\times 5+3}\left(\begin{matrix} 1, 2, 3, 4, 5 \\ i, -2, 2\sqrt{2}, 2-2i, 1 \end{matrix}\ ;\ 0\right) = \Delta\left(\begin{matrix} 1, 2, 3 \\ i, -2 \end{matrix}\ ;\ 0\right) = 8 - 3i\ .$$

To compute ϕ_{16} we need to consider the cycle $\sigma = (4, 3, 2, 1, 5)$, so that

$$\begin{aligned}
\phi_{16} &= Q_{0\times 5+4}\left(\begin{matrix} 4, 3, 2, 1, 5 \\ 2\sqrt{2}, -2, i, 1, 2-2i \end{matrix}\ ;\ 0\right) = \Delta\left(\begin{matrix} 4, 3, 2, 1 \\ 2\sqrt{2}, -2, i \end{matrix}\ ;\ 0\right) \\
&= (32 - 4\sqrt{2}) - i\,(12 - 2\sqrt{2})\ .
\end{aligned}$$

Therefore,

$$\begin{aligned}
(A^{-1})_{15,4} &= \frac{-64\,\theta_3\,\phi_{16}}{\theta_{19}} \\
&= -\frac{538720642301203 + 238439657119632\sqrt{2}}{16363289647822290099} \\
&\quad -i\,\frac{257831938678629 + 60369019908005\sqrt{2}}{16363289647822290099} \\
&= -0.00535299 - 0.000209742\,i\ .
\end{aligned}$$

Next we compute $(A^{-1})_{7,7}$. We need to find θ_6 and ϕ_8. Again by Theorem 4.1,

$$\theta_6 = Q_{1\times 5+1}\begin{pmatrix} 1,2,3,4,5 \\ i,-2,2\sqrt{2},2-2i,1 \end{pmatrix}; 0\Big)$$

$$= U_{1,5}\left(\begin{matrix} 1,2,3,4,5 \\ i,-2,2\sqrt{2},2-2i,1 \end{matrix}; 0\right) + i\,\Delta\left(\begin{matrix} 3,4 \\ 2\sqrt{2} \end{matrix}; 0\right)$$

$$= (118-16\sqrt{2}) - i\,(26-8\sqrt{2})\,,$$

and

$$\phi_8 = Q_{2\times 5+2}\left(\begin{matrix} 4,3,2,1,5 \\ 2\sqrt{2},-2,i,1,2-2i \end{matrix}; 0\right)$$

$$= \Delta\left(\begin{matrix} 4,3 \\ 2\sqrt{2} \end{matrix}; 0\right) U_{2,5}\left(\begin{matrix} 4,3,2,1,5 \\ 2\sqrt{2},-2,i,1,2-2i \end{matrix}; 0\right)$$

$$-8\sqrt{2}(1-i)\,\Delta\left(\begin{matrix} 1 \\ - \end{matrix}; 0\right) U_{1,5}\left(\begin{matrix} 4,3,2,1,5 \\ 2\sqrt{2},-2,i,1,2-2i \end{matrix}; 0\right)$$

$$= (165632-62320\sqrt{2}) - i\,(130048-63472\sqrt{2})\,,$$

hence

$$(A^{-1})_{7,7} = \frac{\theta_6\,\phi_8}{\theta_{19}} = 0.28809 + 0.133898\,i\ .$$

Remark In the above computations, corresponding to a matrix of order $N = 19$ with $k = 5$, we just needed to compute determinants of order 5 (to find $\pi_5(\cdot;0)$) and at most of order 4 (to compute the $\Delta(\cdot;0)$'s determinants), and only values of Chebyschev polynomials of degree at most 3 were needed. This is important from computational aspects. As a matter of fact, in the general case of a $k-$Toeplitz matrix of order N, in order to apply the formulas in Theorem 4.1 to find any specific element of the matrix A^{-1}, we only have to compute

(i) a determinant of order at most k (to find the value of $\pi_k(\cdot;0)$);
(ii) some determinants of order at most $k-1$ (to compute the $\Delta(\cdot;0)$'s determinants);
(iii) and some values of Chebyshev polynomials of degree at most $\lfloor N/k \rfloor$—but we also notice that from the explicit formulas for the Chebyschev polynomials (cf. (2.4)), the computation of $U_{\lfloor N/k \rfloor}$ only requires to sum $1 + \lfloor \lfloor N/k \rfloor /2 \rfloor$ terms.

Henceforth, if N is large enough, and if a "good relation" exists between N and k, then the determinants that we have to compute, as well as the degree of the involved Chebyshev polynomials of the second degree, may be very lower when compared with N. For instance, if $N = 5000$ and $k = 70$, so that $\lfloor N/k \rfloor = 71$, then we only have to compute determinants of order at most 70 and values of Chebyshev polynomials of degree at most 71 (which only involve at most 36 summands).

5 Some remarks on invertibility conditions

Our aim, in this section, is to give some information about invertibility conditions for the $k-$Toeplitz matrix A. In what follows we put

$$b := \prod_{i=1}^{k} b_i \,, \quad c := \prod_{i=1}^{k} c_i \,, \quad \mu^2 := bc \,.$$

For $j > i$, define

$$\Delta_{i,j}(x) := \begin{vmatrix} x-a_i & 1 & 0 & \cdots & 0 & 0 \\ b_i c_i & x-a_{i+1} & 1 & \cdots & 0 & 0 \\ 0 & b_{i+1}c_{i+1} & x-a_{i+2} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & x-a_{j-1} & 1 \\ 0 & 0 & 0 & \cdots & b_{j-1}c_{j-1} & x-a_j \end{vmatrix} ,$$

so that $\Delta_{i,j}$ is a polynomial of degree $j-i+1$ in x, and for $j \le i$ set

$$\Delta_{i,j}(x) := \begin{cases} 0 & \text{if } j < i-1 \\ 1 & \text{if } j = i-1 \\ x-a_i & \text{if } j = i \,. \end{cases}$$

We also define the following polynomial of degree k

$$\varphi_k(x) := \frac{1}{2\mu} \left\{ D_k(x) + (-1)^k \left(b_k c_k + \mu^2/(b_k c_k) \right) \right\} ,$$

where D_k is a monic polynomial of degree k,

$$D_k(x) := \begin{vmatrix} x-a_1 & 1 & 0 & \cdots & 0 & 1 \\ b_1 c_1 & x-a_2 & 1 & \cdots & 0 & 0 \\ 0 & b_2 c_2 & x-a_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & x-a_{k-1} & 1 \\ b_k c_k & 0 & 0 & \cdots & b_{k-1}c_{k-1} & x-a_k \end{vmatrix} .$$

It is important to keep in mind that in what follows we consider that these polynomials φ_k and D_k are defined only when $k \geq 3$. We begin by pointing out that, up to a constant factor the characteristic polynomial for A, $p(x;\, A) := \det(xI_N - A)$, I_N being the identity matrix of order N, is obtained by an affine change in the variable in the polynomial Q_N, introduced in the previous section, corresponding to the entries which appear in A.

Theorem 5.1 *Assume that the tridiagonal $k-$Toeplitz matrix A of order N is irreducible, with $k \geq 3$. Then its characteristic polynomial is*

$$p(x;\, A) = (-1)^N\, Q_N \left(\begin{matrix} a_1, \cdots, a_k \\ b_1c_1, \cdots, b_kc_k \end{matrix} \,;\, -x \right).$$

Alternatively, r being characterized by $0 \leq r \leq k-1$ and $N \equiv r \,(\mathrm{mod}\, k)$,

$$\begin{aligned} p(x;\, A) = \mu^{\lfloor N/k \rfloor} \Big\{ & \Delta_{1,r}(x)\, U_{\lfloor N/k \rfloor}(\varphi_k(x)) \\ & + \tfrac{b_kc_k}{\mu} \left(\textstyle\prod_{i=1}^{r} b_ic_i \right) \Delta_{r+2,k-1}(x)\, U_{\lfloor (N-k)/k \rfloor}(\varphi_k(x)) \Big\}. \end{aligned}$$

In particular, if $N \equiv (k-1)\,(\mathrm{mod}\, k)$, then

$$p(x;\, A) = \mu^{\lfloor N/k \rfloor}\, \Delta_{1,k-1}(x)\, U_{\lfloor N/k \rfloor}(\varphi_k(x)),$$

and the eigenvalues of A are the $k-1$ zeros of $\Delta_{1,k-1}(x)$ together with all the solutions of the following $\lfloor N/k \rfloor$ algebraic equations of degree k

$$\varphi_k(x) = \cos \frac{jk\pi}{N+1}, \quad j = 1, 2, \cdots, \lfloor N/k \rfloor.$$

Proof First, remark that

$$A = D^{-1} J_N D,$$

where D is a diagonal matrix of order N,

$$D := \mathrm{diag}\,\{d_1, d_2, \cdots, d_N\}, \quad d_{nk+i} := \left(\prod_{s=1}^{i-1} b_s \right) \left(\prod_{s=1}^{k} b_s \right)^n$$

$(1 \leq i \leq k;\, n = 0, 1, \cdots, \lfloor N/k \rfloor)$, and J_N is the tridiagonal $k-$Toeplitz matrix

$$J_N := \begin{pmatrix} a_1 & 1 & & & & & & & & & \\ b_1c_1 & \ddots & \ddots & & & & & & & & \\ & \ddots & a_k & 1 & & & & & & & \\ & & b_kc_k & a_1 & 1 & & & & & & \\ & & & b_1c_1 & \ddots & \ddots & & & & & \\ & & & & \ddots & a_k & 1 & & & & \\ & & & & & b_kc_k & a_1 & 1 & & & \\ & & & & & & b_1c_1 & \ddots & \ddots & & \\ & & & & & & & \ddots & & & \end{pmatrix} \in \mathbb{C}^{N\times N}.$$

Now notice that J_N is the Jacobi matrix of order N corresponding to the MOPS $\{(-1)^n p_n(-x)\}_{n\geq 0}$, where $\{p_n(x)\}_{n\geq 0}$ is the MOPS generated by the block of recurrence relations (2.6) with $\{a_n^{(j)}\}$ and $\{b_n^{(j)}\}$ defined by (4.29). We have seen in the proof of Theorem 4.1 that this sequence $\{p_n(x)\}_{n\geq 0}$ is determined by (4.32). Hence since A and J_N are similar matrices, and the characteristic polynomial of J_N is $(-1)^N p_N(-x)$, it follows that

$$p(x;A) = (-1)^N p_N(-x) = (-1)^N Q_N \left(\begin{matrix} a_1, \cdots, a_k \\ b_1c_1, \cdots, b_kc_k \end{matrix} ; -x \right).$$

The alternative expression for $p(x;A)$ stated in the theorem comes now easily taking into account the definition of Q_N in terms of the Chebyshev polynomials of the second kind as well as the relations

$$\begin{aligned} &(-1)^k \pi_k \left(\begin{matrix} a_1, \cdots, a_k \\ b_1c_1, \cdots, b_kc_k \end{matrix} ; -x \right) + b_kc_k + \mu^2/(b_kc_k) \\ &\quad = D_k(x) + (-1)^k \left(b_kc_k + \mu^2/(b_kc_k) \right), \end{aligned} \tag{5.36}$$

$$\Delta_{i,j}(x) = (-1)^{j-i+1}\, \Delta \left(\begin{matrix} a_i, a_{i+1}, \cdots, a_j \\ b_ic_i, b_{i+1}c_{i+1}, \cdots, b_{j-1}c_{j-1} \end{matrix} ; -x \right)$$

and $U_m(x) = (-1)^m U_m(-x)$. The formula given for the case $N \equiv (k-1) \bmod k$, i.e., $r = k-1$, is a consequence of the general formula since $\Delta_{k+1,k-1}(x) \equiv 0$; and the algebraic equations for the determination of the eigenvalues follows from the trigonometric expression for the Chebyshev polynomials of the second kind. □

Remark We have proved the preceding theorem assuming $k \geq 3$. However, a direct inspection of the proofs in the previous theorems shows that the second expression for $p(x;A)$ (and the formulas after it) remains valid for $k=1$ and $k=2$ provided one defines

$$\varphi_1(x) := \frac{1}{2\mu}\,(x-a_1)\,,$$
$$\varphi_2(x) := \frac{1}{2\mu}\,\{\,(x-a_1)(x-a_2)-(b_1c_1+b_2c_2)\,\}\,.$$

(In fact, this can easily be seen by comparing the relation $(-1)^k T(-x) = 2\mu\varphi_k(x)$, which is true for $k\geq 3$ – according to (4.31) and (5.36) – with the definition (4.30) of T, which is valid for any $k\geq 1$.) As a consequence, we conclude that Theorem 5.1 recovers and generalizes results from [5], [9], [19] and [20], where the characteristic polynomial of A has been computed is some special situations. In fact, the cases $r=0$ and $r=k-1$ (for arbitrary k) have been treated in [5]; the case $k=2$ in [9] and [19], but we notice that this is a particular situation of the cases treated in [5]; and the solution for the case $k=3$ have been presented in [21] (which only partially follows from [5]).

From Theorem 5.1 we get

$$\det A = (-1)^N\, p(0;A) = Q_N\left(\begin{matrix} a_1,\cdots,a_k \\ b_1c_1,\cdots,b_kc_k\end{matrix}\,;\,0\right)\,,$$

or

$$\begin{aligned}\det A = {}& (-1)^N\,\mu^{\lfloor N/k\rfloor}\,\Big\{\,\Delta_{1,r}(0)\,U_{\lfloor N/k\rfloor}\,(\varphi_k(0)) \\ & + \tfrac{b_kc_k}{\mu}\,\left(\textstyle\prod_{i=1}^r b_ic_i\right)\,\Delta_{r+2,k-1}(0)\,U_{\lfloor (N-k)/k\rfloor}\,(\varphi_k(0))\,\Big\}\,.\end{aligned}$$

Hence, it follows that A is nonsingular if and only if

$$Q_N\left(\begin{matrix} a_1,\cdots,a_k \\ b_1c_1,\cdots,b_kc_k\end{matrix}\,;\,0\right)\neq 0\,,$$

which, of course, can be reformulated in terms of the second expression for $\det A$. In particular, when $N\equiv(k-1)(\mathrm{mod}\,N)$ then A^{-1} exists if and only if

$$\Delta_{1,k-1}(0)\neq 0\,,\quad \varphi_k(0)\neq\cos\frac{jk\pi}{N+1}\,,\qquad j=1,2,\cdots,\lfloor N/k\rfloor\,.$$

Consider again an arbitrary N and assume that the conditions

$$\Delta_{1,r}(0)\neq 0\,,\quad \varphi_k(0)\notin[-1,1] \tag{5.37}$$

hold (the last one ensures that $U_s(\varphi_k(0))\neq 0$ for all s). Then the quantity

$$\eta(A) := -\,\tfrac{b_kc_k}{\mu}\,\left(\textstyle\prod_{i=1}^r b_ic_i\right)\,\frac{\Delta_{r+2,k-1}(0)}{\Delta_{1,r}(0)}$$

is effectively computable and from the above expression for det A we find that A is nonsingular if and only if

$$\eta(A) \neq \frac{U_{\lfloor N/k \rfloor}(\varphi_k(0))}{U_{\lfloor (N-k)/k \rfloor}(\varphi_k(0))} \, .$$

This and (2.5) enable us to state the following asymptotic result: under conditions (5.37), for N large enough A^{-1} exists provided that

$$\eta(A) \neq \varphi_k(0) + \sqrt{\varphi_k^2(0) - 1} \, ,$$

where the square root is taken in the same sense as in (2.5).

Remark The characteristic polynomial $\Phi_N(\cdot;\, J)$ of the general tridiagonal matrix J in (3.15) has been computed in [18], as an explicit expression in terms of the entries of the matrix J. It reads as (cf. (80a) in [18])

$$\Phi_N(x;\, J) = (x-\beta_1)\cdots(x-\beta_N) \times \left(1 + \sum_{q=1}^{\lfloor N/2 \rfloor} \sum_{(k_1,\cdots,k_q)\in S_q(2,N)} \eta_{k_1}(x)\cdots\eta_{k_q}(x)\right) \, ,$$

where

$$\eta_\ell(x) := -\frac{\alpha_{\ell-1}\gamma_{\ell-1}}{(x-\beta_{\ell-1})(x-\beta_\ell)} \quad (\ell = 2, \cdots, N) \, .$$

Regarded from the view point of orthogonal polynomials, it is clear that this formula gives a general explicit expression for the monic orthogonal polynomial of degree N, of any given system of orthogonal polynomials, only in terms of the coefficients in the three-term recurrence relation characterizing this system. When J becomes the tridiagonal $k-$Toeplitz matrix A in (1.1) one has $\Phi_N(x;\, J) = p(x;\, A)$, and the conjugation of the above expression for $\Phi_N(x;\, J)$ (in this specific case $J = A$) with the expression for $p(\cdot;\, A)$ as in Proposition 5.1 leads to closed formulae to compute the above intricate sum involving the set $S_q(2, N)$. In the particular case when $N \equiv (k-1) \bmod k$, one gets

$$\sum_{q=1}^{\lfloor N/2 \rfloor} \sum_{(k_1,\cdots,k_q)\in S_q(2,N)} (-1)^q \prod_{s=1}^{q} \frac{b_{k_s-1}\, c_{k_s-1}}{(x-a_{k_s-1})(x-a_{k_s})} = \frac{\mu^{\lfloor N/k \rfloor}\, \Delta_{1,k-1}(x)\, U_{\lfloor N/k \rfloor}\, (\varphi_k(x))}{(x-a_1)\cdots(x-a_N)} - 1 \, .$$

Giving concrete values to the variable x, as well as to the involved parameters, many identities can be obtained as special cases of these kind of formulae (for instance, conjugating the explicit expressions for the entries of A^{-1} given by the two approaches) for computing sums involving the sets $S_q(L, U)$. We believe that this may leads to interesting combinatorial-type identities, as well as corresponding combinatorial interpretations.

Acknowledgements. The authors would like to thank the anonymous referees for the many valuable comments and references.

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