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ORIGINAL PAPER

On the determinant evaluation of quasi penta-diagonal matrices and quasi penta-diagonal Toeplitz matrices

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Abstract Recently, three computational algorithms for evaluating the determinant of quasi penta-diagonal matrices have been proposed by El-Mikkawy and Rahmo (Comput Math Appl 59:1386–1396, 2010), by Neossi Nguetchue and Abelman (Appl Math Comput 203:629–634, 2008), and by Jia et al. (Int J Comput Math 89:851–860, 2013), respectively. In the current paper, two novel algorithms with less computational costs are proposed for the determinant evaluation of general quasi penta-diagonal matrices and quasi penta-diagonal Toeplitz matrices. Furthermore, three numerical experiments are given to show the performance of our algorithms. All of the numerical computations were performed on a computer with aid of programs written in MATLAB.

Keywords Quasi penta-diagonal matrix · Toeplitz matrix · Triangular matrix · Determinant · Computational costs

1 Introduction and objectives

Penta-diagonal matrices and quasi penta-diagonal matrices frequently occur in several mathematical chemistry [1,2] as well as scientific and engineering investigations

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[3–6]. In quantum chemistry, finite difference methods using quasi penta-diagonal matrices are used both in the wavefunction formalism [7] and density functional theory [8]. Because of their simplicity and importance in many applications, these types of matrices have been thoroughly studied in the past decades [9–20].

In this paper, we mainly consider the n-by-n quasi penta-diagonal matrix given by

$$A := \begin{pmatrix} D & F \\ G & P \end{pmatrix}, \tag{1.1}$$

where

$$\begin{aligned} D &:= \begin{pmatrix} d_1 & a_1 \\ b_2 & d_2 \end{pmatrix}, \\ F &:= \begin{pmatrix} c_1 & 0 & \cdots & 0 & e_1 & b_1 \\ a_2 & c_2 & 0 & \cdots & 0 & e_2 \end{pmatrix} \in \mathbb{R}^{2\times(n-2)}, \\ G &:= \begin{pmatrix} e_3 & 0 & \cdots & 0 & c_{n-1} & a_n \\ b_3 & e_4 & 0 & \cdots & 0 & c_n \end{pmatrix}^T \in \mathbb{R}^{(n-2)\times 2}, \end{aligned}$$

and P is an $(n-2)$-by-$(n-2)$ penta-diagonal matrix takes the form

$$P := \begin{pmatrix} d_3 & a_3 & c_3 & & & \\ b_4 & d_4 & a_4 & \ddots & & \\ e_5 & b_5 & \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots & \ddots & c_{n-2} \\ & & \ddots & \ddots & \ddots & a_{n-1} \\ & & & e_n & b_n & d_n \end{pmatrix}. \tag{1.2}$$

In addition, as an important subclass of the quasi penta-diagonal matrices, a quasi penta-diagonal Toeplitz matrix $\tilde{A}$ can be obtained by setting $d_i = d$, $a_i = a$, $b_i = b$, $c_i = c$, $e_i = e$, for $i = 1, 2, \ldots, n$ in (1.1), thus

$$\tilde{A} = \begin{pmatrix} d & a & c & & e & b \\ b & d & a & c & & e \\ e & b & \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots & \ddots & c \\ c & & \ddots & \ddots & d & a \\ a & c & & e & b & d \end{pmatrix}. \tag{1.3}$$

From practical point of view, usually, a fast and reliable algorithm for computing $\det(A)$ (or $\det(\tilde{A})$) is linked to the problem of obtaining efficient test for the existence of unique solution of the corresponding system. Therefore, in order to evaluate the determinant of the quasi penta-diagonal matrices, some researchers have derived symbolic or numerical algorithms recently. For example, El-Mikkawy and Rahmo [12], Neossi Nguetchue and Abelman [13], Jia et al. [14]. The motivation of the current paper is to establish some more efficient algorithms for the determinant evaluation of A (1.1) and $\tilde{A}$ (1.3).

The rest of the present paper is organized as follows: in the next section, we present an efficient algorithm for evaluating the determinant of the quasi penta-diagonal matrix based on any penta-diagonal solvers. In Sect. 3, a quasi penta-diagonal Toeplitz matrix is investigated and an approach for the evaluation of its determinant has been described. In Sect. 4, three numerical examples are carried out for the sake of illustration, and finally, some concluding remarks are given in Sect. 5.

2 A determinant evaluation for the quasi penta-diagonal matrix

It follows from (1.1) and two auxiliary matrices

$$E := (\mathbf{e}_1, \mathbf{e}_2) = \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 \end{pmatrix}^T \in \mathbb{R}^{n\times 2}, \tag{2.1}$$

$$V := \begin{pmatrix} d_1 - 1 & a_1 & c_1 & 0 & \cdots & 0 & e_1 & b_1 \\ b_2 & d_2 - 1 & a_2 & c_2 & 0 & \cdots & 0 & e_2 \end{pmatrix} \in \mathbb{R}^{2\times n} \tag{2.2}$$

that the matrix A can be rewritten by the following form

$$A = \bar{A} + EV = \begin{pmatrix} I_2 & O \\ G & P \end{pmatrix} + EV, \tag{2.3}$$

where I_2 is an 2-by-2 identity matrix.

Theorem 2.1 (Sylvester's determinant theorem) *Let X be an m-by-n matrix, Y an n-by-m matrix. Then*

$$det(I_m + XY) = det(I_n + YX),$$

where I_m and I_n denote the m-by-m and n-by-n identity matrix respectively.

We now give a determinant evaluation for A (1.1) below.

Theorem 2.2 *Let A be a quasi penta-diagonal matrix, $\bar{A}$ and P be matrices given in (2.3). Let U and V be matrices of the form $\bar{A}^{-1}E$ and (2.2), respectively. Then, the determinant of A is given by*

$$det(A) = det(P) \cdot det(I_2 + VU).$$

Proof It follows from (2.3) that the matrix A can be split by

$$A = \bar{A} + EV,$$

then we readily have

$$\det(A) = \det(\bar{A} + EV) = \det(\bar{A}) \cdot \det(I_n + \bar{A}^{-1}EV).$$

Since the matrix $\bar{A}$ can be factorized as

$$\bar{A} = L\tilde{P} = \begin{pmatrix} I_2 & O \\ G & I_{n-2} \end{pmatrix} \begin{pmatrix} I_2 & O \\ O & P \end{pmatrix}, \tag{2.4}$$

where I_{n-2} is an $(n-2)$-by-$(n-2)$ identity matrix, it is easy to see that

$$\det(\bar{A}) = \det(P).$$

On the other hand, by using Theorem 2.1, we have

$$\det(I_n + \bar{A}^{-1}EV) = \det(I_2 + V\bar{A}^{-1}E).$$

Thus,

$$\det(A) = \det(P) \cdot \det(I_2 + VU).$$ □

From the theorem above, it is necessary to compute $U = [\mathbf{u}_1, \mathbf{u}_2] = \bar{A}^{-1}E$. With the factorization of $\bar{A}$ in (2.4), the matrix U can be obtained by solving the following linear systems:

$$\tilde{P}[\mathbf{u}_1, \mathbf{u}_2] = [L^{-1}\mathbf{e}_1, L^{-1}\mathbf{e}_2], \tag{2.5}$$

where $L^{-1} = \begin{pmatrix} I_2 & O \\ -G & I_{n-2} \end{pmatrix}$.

In fact, by some simple matrix-vector multiplications, one may compute the right-hand sides of the systems above immediately. Since P is a penta-diagonal matrix, the linear systems (2.5) can be efficiently solved by any penta-diagonal solver.

Below, we state an algorithm for evaluating the determinant of the quasi penta-diagonal matrix A (1.1).

Algorithm 2.1

Step1. Input $\tilde{P}, L, V, E$ and n.
Step2. Solve $\tilde{P}[\mathbf{u}_1, \mathbf{u}_2] = [\tilde{L}^{-1}\mathbf{e}_1, \tilde{L}^{-1}\mathbf{e}_2]$ by using any penta-diagonal solver.
Step3. Compute $\det(P)$ and $\det(I_2 + VU)$.
Step4. Output the determinant: $\det(A) = \det(P) \cdot \det(I_2 + VU)$.

Let us calculate the computational costs of the algorithm above. In Step 2, it takes $26n - 87$ operations for obtaining $\mathbf{u}_1, \mathbf{u}_2$ if we use Crout LU decomposition and forward substitution and back substitution, for details, see [21]. Furthermore, since costs for the Step 3 and 4 are $n + 27$ and 1 respectively, we need $27n - 59$ operations to compute the determinant of A. We provide a comparison of the total operations

Table 1 Total operations for the determinant of a quasi penta-diagonal matrix

	Algorithm 1 [12,13]	Algorithm 2 [14]	Our algorithm
Total operations	$36n - 102$	$33n + 4$	$27n - 59$

among DETCPENTA algorithm [12], NPENTA algorithm [13], Jia et al.'s algorithm [14] and our algorithm in the following table. Algorithm 2.1 will be referred to as the DETQP algorithm (Table 1).

3 An approach for the quasi penta-diagonal matrix with Toeplitz structure

In this section, we first give an approach for the determinant of a penta-diagonal Toeplitz matrix. Then, based on the proposed approach, a numerical algorithm for evaluating the determinant of a quasi penta-diagonal Toeplitz matrix is presented.

3.1 Determinant of a penta-diagonal Toeplitz matrix

Let the penta-diagonal Toeplitz matrix

$$T = \begin{pmatrix} d & a & c & & \\ b & d & a & \ddots & \\ e & b & d & \ddots & c \\ & \ddots & \ddots & \ddots & a \\ & & e & b & d \end{pmatrix} \in \mathbb{R}^{n\times n}. \tag{3.1}$$

Throughout this paper, we suppose that T is nonsingular and the element c satisfies $c \neq 0$.

Theorem 3.1 *Let T be an n-by-n penta-diagonal Toeplitz matrix. Then*

$$det(T) = c^{n-2} \cdot det(S),$$

where

$$S = \begin{pmatrix} em_{n-4} + bm_{n-3} + dm_{n-2} + am_{n-1} & em_{n-5} + bm_{n-4} + dm_{n-3} + am_{n-2} \\ em_{n-3} + bm_{n-2} + dm_{n-1} & em_{n-4} + bm_{n-3} + dm_{n-2} \end{pmatrix},$$

and $\{m_i\}_{1\leq i\leq n-1}$ is the sequence defined by the recurrence relation

$$\frac{e}{c}m_{i-4} + \frac{b}{c}m_{i-3} + \frac{d}{c}m_{i-2} + \frac{a}{c}m_{i-1} + m_i = 0, \tag{3.2}$$

for $i = 5, 6, \ldots, n-1$, *and* $m_1 = -\frac{a}{c}, m_2 = -\frac{d+am_1}{c}, m_3 = -\frac{b+dm_1+am_2}{c}$, $m_4 = -\frac{e+bm_1+dm_2+am_3}{c}$.

Proof Let X be an n-by-n lower triangular matrix of the form

$$X = \begin{pmatrix} 1 & & & & & \\ m_1 & 1 & & & & \\ m_2 & m_1 & 1 & & & \\ \vdots & \vdots & 0 & \ddots & & \\ m_{n-2} & m_{n-3} & \vdots & \ddots & \ddots & \\ m_{n-1} & m_{n-2} & 0 & \cdots & 0 & 1 \end{pmatrix}.$$

Partition T as

$$T = \begin{pmatrix} W & Y \\ O & Z \end{pmatrix},$$

where W, Y, Z are matrices of size $(n-2) \times 2, (n-2) \times (n-2), 2 \times (n-2)$, respectively. Then, by relation (3.2) and some simple matrices multiplications, we can obtain

$$TX = \begin{pmatrix} O & Y \\ S & Z \end{pmatrix},$$

where

$$S = \begin{pmatrix} em_{n-4} + bm_{n-3} + dm_{n-2} + am_{n-1} & em_{n-5} + bm_{n-4} + dm_{n-3} + am_{n-2} \\ em_{n-3} + bm_{n-2} + dm_{n-1} & em_{n-4} + bm_{n-3} + dm_{n-2} \end{pmatrix}.$$

Hence, it follows that

$$\det(T) = \det(TX) = \det(Y) \cdot \det(S) = c^{n-2} \cdot \det(S),$$

since $\det(X) = 1$. The result follows. □

Remark 3.1 The complexity of the approach above are $8n + 10$, since it takes $7n + 12$ operations for obtaining $\det(S)$, and c^{n-2} can be computed in $n - 3$ operations. In addition, for computing the determinant of a penta-diagonal Toeplitz matrix, the algorithms given in [15–17,19,20] require $24n - 59, 22n - 50, 14n - 28, 11n - 17, 9n + 3$ operations, respectively.

3.2 An efficient algorithm for evaluating the determinant of a quasi penta-diagonal Toeplitz matrix

In this subsection, we study on the determinant of the quasi penta-diagonal Toeplitz matrix $\tilde{A}$ given in (1.3).

Consider the following $(n+2)$-by-$(n+2)$ lower triangular Toeplitz matrix

$$\tilde{L} = \begin{pmatrix} c & & & & & & \\ a & c & & & & & \\ d & a & \ddots & & & & \\ b & \ddots & \ddots & \ddots & & & \\ e & \ddots & \ddots & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & a & c & \\ & & e & b & d & a & c \end{pmatrix} = \begin{pmatrix} Q_1 & O \\ T & Q_2 \end{pmatrix}, \tag{3.3}$$

where

$$Q_1 = \begin{pmatrix} c & 0 & 0 & \cdots & 0 \\ a & c & 0 & \cdots & 0 \end{pmatrix} \in \mathbb{R}^{2\times n},$$

$$Q_2 = \begin{pmatrix} 0 & \cdots & 0 & c & a \\ 0 & \cdots & 0 & 0 & c \end{pmatrix}^T \in \mathbb{R}^{n\times 2}.$$

Let the first column of $\tilde{L}^{-1}$ is $(\eta_1, \eta_2, \ldots, \eta_{n+2})^T$ and $\eta_i = 0$ for $i \leq 0$. Then, the following theorem has recently been proved in [17].

Theorem 3.2 *Let T be an n-by-n penta-diagonal Toeplitz matrix and $\tilde{L}$ be its associated lower triangular matrix as in (3.3), $(\eta_1, \eta_2, \ldots, \eta_{n+2})^T$ is the first column of $\tilde{L}^{-1}$, then $T^{-1} = (t_{i,j})$ exists and*

$$t_{i,j} = \frac{\eta_i(\eta_{n+1}\eta_{n-j} - \eta_n\eta_{n+1-j}) + \eta_{i-1}(-\eta_{n+2}\eta_{n-j} + \eta_{n+1}\eta_{n+1-j})}{\eta_n\eta_{n+2} - \eta_{n+1}^2} + \eta_{i-j-1}. \tag{3.4}$$

Proof See, e.g., [17]. □

Hence, it is important to compute the elements η_i $(i = 1, 2, \ldots, n+2)$ in the first column of $\tilde{L}^{-1}$. After solving $\tilde{L}\eta = \mathbf{e}_1$ by using the forward substitution, we can obtain the general recurrence formula

$$\eta_i = -\sum_{j=1}^{i-1} r_{j-i}\eta_j, \ i = 2, 3, \ldots, n+2, \tag{3.5}$$

where $\eta_1 = \frac{1}{c}$, $r_0 = 1$, $r_{-1} = \frac{a}{c}$, $r_{-2} = \frac{d}{c}$, $r_{-3} = \frac{b}{c}$, $r_{-4} = \frac{e}{c}$ and $r_k = 0$ for $k < 0$.

Let $\hat{T}$ be the $(n-2)$-by-$(n-2)$ leading principal submatrix of $\tilde{A}$ (1.3). Then, matrix $\tilde{A}$ can be partitioned as

$$\tilde{A} = \begin{pmatrix} \hat{T} & B \\ C & D \end{pmatrix}, \ B \in \mathbb{R}^{(n-2)\times 2}, \ C \in \mathbb{R}^{2\times(n-2)}, \ D \in \mathbb{R}^{2\times 2}.$$

From the Aitken block-diagonalization formula [22],

$$\begin{pmatrix} \hat{T} & B \\ C & D \end{pmatrix} = \begin{pmatrix} I_{n-2} & O \\ C\hat{T}^{-1} & I_2 \end{pmatrix} \begin{pmatrix} \hat{T} & O \\ O & \hat{E} \end{pmatrix} \begin{pmatrix} I_{n-2} & \hat{T}^{-1}B \\ O & I_2 \end{pmatrix},$$

where $\hat{E} = D - C\hat{T}^{-1}B$, we obtain

$$\begin{aligned} \det(\tilde{A}) &= \det\left(\begin{pmatrix} I_{n-2} & O \\ C\hat{T}^{-1} & I_2 \end{pmatrix} \begin{pmatrix} \hat{T} & O \\ O & \hat{E} \end{pmatrix} \begin{pmatrix} I_{n-2} & \hat{T}^{-1}B \\ O & I_2 \end{pmatrix}\right) \\ &= \det\begin{pmatrix} \hat{T} & O \\ O & \hat{E} \end{pmatrix} = \det(\hat{T}) \cdot \det(\hat{E}). \end{aligned}$$

Hence, by using Theorem 3.1, it yields

$$\det(\tilde{A}) = c^{n-4} \cdot \det(S) \cdot \det(\hat{E}). \tag{3.6}$$

Moreover, based on the special structure of B and C, it follows that

$$\hat{E} = D - (C_1\ C_2)\tilde{T}\begin{pmatrix} C_2 \\ C_1 \end{pmatrix}, \tag{3.7}$$

where

$$C_1 = \begin{pmatrix} c & 0 \\ a & c \end{pmatrix},\ C_2 = \begin{pmatrix} e & b \\ 0 & e \end{pmatrix},$$

and

$$\tilde{T} = \begin{pmatrix} t_{1,1} & t_{1,2} & t_{1,n-3} & t_{1,n-2} \\ t_{2,1} & t_{2,2} & t_{2,n-3} & t_{2,n-2} \\ t_{n-3,1} & t_{n-3,2} & t_{n-3,n-3} & t_{n-3,n-2} \\ t_{n-2,1} & t_{n-2,2} & t_{n-2,n-3} & t_{n-2,n-2} \end{pmatrix}.$$

The elements of $\tilde{T}$ can be obtained by using (3.4).

In the following, we give an algorithm for evaluating the determinant of a quasi penta-diagonal Toeplitz matrix $\tilde{A}$ as in (1.3).

Algorithm 3.1

Step1. Input a, b, c, d, e and n.
Step2. Compute $m_1, m_2, \ldots, m_{n-3}$ by using (3.2), then obtain the matrix S in Theorem 3.1.
Step3. Compute $\eta_1, \eta_2, \ldots, \eta_n$ by using (3.5), then obtain the matrix $\tilde{T}$.
Step4. Compute $\hat{E}$ by using (3.7).
Step5. Output the determinant: $\det(\tilde{A}) = c^{n-4} \cdot \det(S) \cdot \det(\hat{E})$.

This algorithm will be referred to as the DETQPT algorithm. In addition, the total operations of Algorithm 3.1 are $15n + 184$, since costs for the Step 2, 3, 4 and 5 are $7n - 5$, $7n + 122$, 64 and $n + 3$, respectively.

Remark 3.2 It should be mentioned that since c^{n-4} can be computed in $O(\log n)$ operations, see [23], the algorithm above may give $\det(\tilde{A})$ in $14n+O(\log n)$ operations.

4 Numerical examples

In order to illustrate the performance of our algorithm, we give the results of three simple numerical examples in this section. All numerical experiments were performed in MATLAB 7.12.0.635 (R2011a).

Example 4.1 First, we compute the determinant of an 7-by-7 quasi penta-diagonal matrix originating from [12]

$$A = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 1 & 2 \\ 1 & 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 2 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 2 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 2 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 & 2 & 2 \\ 2 & 1 & 0 & 0 & 1 & 2 & 2 \end{pmatrix}.$$

Since

$$P = \begin{pmatrix} 2 & 1 & 1 & 0 & 0 \\ 1 & 2 & 1 & 1 & 0 \\ 1 & 1 & 2 & 1 & 1 \\ 0 & 1 & 1 & 2 & 2 \\ 0 & 0 & 1 & 2 & 2 \end{pmatrix}, \quad V = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 1 & 2 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

By using Algorithm 2.1, we can compute

$$U = \begin{pmatrix} 1.0000 & 0.0000 & -1.5000 & 1.0000 & 1.0000 & -1.5000 & 0.0000 \\ 0.0000 & 1.0000 & -1.2500 & 1.0000 & 0.5000 & -1.2500 & 0.5000 \end{pmatrix}^T.$$

Thus, $\det(A) = \det(P) \cdot \det(I_2 + VU) = 3.0000$. It should be mentioned that the determinant of matrix A given by MATLAB "`det(A)`" is 3.

Example 4.2 Next, we consider the following 7-by-7 quasi penta-diagonal Toeplitz matrix

$$A = \begin{pmatrix} 1 & -1 & 2 & 0 & 0 & 3 & -2 \\ -2 & 1 & -1 & 2 & 0 & 0 & 3 \\ 3 & -2 & 1 & -1 & 2 & 0 & 0 \\ 0 & 3 & -2 & 1 & -1 & 2 & 0 \\ 0 & 0 & 3 & -2 & 1 & -1 & 2 \\ 2 & 0 & 0 & 3 & -2 & 1 & -1 \\ -1 & 2 & 0 & 0 & 3 & -2 & 1 \end{pmatrix}.$$

By using Algorithm 3.1, we obtain

$$S = \begin{pmatrix} 3.1875 & 1.1250 \\ -2.5625 & 2.6250 \end{pmatrix}, \hat{E} = \begin{pmatrix} -8.6222 & 5.8222 \\ 1.8222 & -8.6222 \end{pmatrix}.$$

Then, we can compute $\det(A) = 2^3 \cdot \det(S) \cdot \det(\hat{E}) = 5736.0000$ by using (3.6). We also note that the determinant of matrix A given by MATLAB "`det(A)`" is 5736.

Example 4.3 Now, we consider an n-by-n quasi penta-diagonal matrix Toeplitz of the form

$$A = \begin{pmatrix} 2.5 & 1.5 & 1 & & & 1 & 1.5 \\ 1.5 & 2.5 & 1.5 & 1 & & & 1 \\ 1 & 1.5 & 2.5 & 1.5 & 1 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & \ddots & 1 \\ 1 & & & 1 & 1.5 & 2.5 & 1.5 \\ 1.5 & 1 & & & 1 & 1.5 & 2.5 \end{pmatrix}.$$

The results with DETCPENTA algorithm [12], NPENTA algorithm [13], Jia et al.'s algorithm [14], MATLAB "`det(A)`" and our algorithms are shown in Table 2. We note from Table 2 that our algorithm generated almost the same value as the others.

5 Concluding remarks

In this paper, we present a numerical algorithm for evaluating the determinant of quasi penta-diagonal matrices. The proposed algorithm leads to a decrease in the number of

Table 2 Numerical results of the determinant for Example 4.3

n	100	1,000	10,000
Algorithm 1 [12,13]	0.05482182545302	4.70260820448565	2.56900241915417
Algorithm 2 [14]	0.05482182545302	4.70260820448583	2.56900241915659
Algorithm 2.1	0.05482182545302	4.70260820448590	2.56900241915641
Algorithm 3.1	0.05482182545301	4.70260820448583	2.56900241915659
MATLAB "`det(A)`"	0.05482182545302	4.70260820448588	2.56900241915650

operations. In fact, we have shown that the total operations of our algorithm (Algorithm 2.1) is less than those of three recent algorithms given in [12–14], when the matrix order $n \geq 5$. Moreover, an efficient algorithm (Algorithm 3.1) for the determinant evaluation of a quasi penta-diagonal Toeplitz matrix has been also derived in Sect. 3. Finally, three numerical examples are given for the sake of illustration.

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