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The Use of the Factorization of Five-Diagonal Matrices by Tridiagonal Toeplitz Matrices

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Abstract—The aim of this paper is the use of the factorization of five-diagonal matrices as the product of two Toeplitz tridiagonal matrices. Either bounds for the inverse or numerical methods for solving linear systems may be derived. Some results will be extended to block five-diagonal matrices. Applications to the numerical solution of ODE and PDE together with numerical tests will be given.

Keywords—Factorization, Toeplitz matrices, Linear systems, Parallel algorithms.

1. INTRODUCTION

Five-diagonal matrices (or block five-diagonal matrices) occur in several fields such as numerical solution of ordinary and partial differential equations (ODE and PDE), interpolation problems, boundary value problems (BVP), etc. In this paper, we will employ the factorization of certain five-diagonal matrices by Toeplitz tridiagonal ones to study bounds for the inverse and in the solution of linear systems. Some of these results will be extended to block five-diagonal matrices. It is known that the product of two tridiagonal Toeplitz matrices is not a Toeplitz five-diagonal matrix because the first and the last element in the principal diagonal are different to the other ones (see [1,2]). However, it is possible the factorization of five-diagonal Toeplitz matrices modified in the first and last element of the principal diagonal.

We begin by considering the class of linear systems

$$Ax = \mathbf{q}, \tag{1}$$

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where $\mathbf{q} \in \mathbf{R}^n$, $A \in \mathbf{R}^{n\times n}$ is the following five-diagonal matrix:

$$A = \begin{pmatrix} x-\alpha & y & v & & & \\ z & x & y & v & & \\ w & z & x & y & v & \\ & \cdot & \cdot & \cdot & \cdot & v \\ & & \cdot & \cdot & x & y \\ & & & w & z & x-\beta \end{pmatrix}. \tag{2}$$

The real tridiagonal Toeplitz matrix of size n given by

$$T = \begin{pmatrix} a & b & & & \\ c & a & b & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & c & a & b \\ & & & c & a \end{pmatrix} \tag{3}$$

will denote by

$$T = \mathrm{trid}_n[c,\ a,\ b].$$

In this paper, we will consider matrices A of the form (2) for which the factorization

$$A = T_1 T_2 \tag{4}$$

exists, with

$$T_1 = \mathrm{trid}_n[c,\ a,\ b], \qquad T_2 = \mathrm{trid}_n\left[c',\ a',\ b'\right]. \tag{5}$$

Then either the solution of linear system (1) or bounds for the inverse may be derived by known results on tridiagonal and block tridiagonal matrices (see [3]). It is easy to verify that the factorization $A = T_1T_2$ exists if and only if the following equations are satisfied:

$$\begin{aligned} aa' + bc' + cb' &= x, \\ ab' + ba' &= y, \\ c' + ca' &= z, \\ bb' &= v, \\ cc' &= w, \\ cb' &= \alpha, \\ bc' &= \beta. \end{aligned} \tag{6}$$

A method for solving (6) has been proposed in [1]: if, for a fixed, the following two equations are satisfied:

$$\begin{gathered} \alpha\beta = vw, \\ s^3 - xs^2 + (yz - 4vw)s - (y^2w + z^2v - 4xvw) = 0 \end{gathered} \tag{7}$$

with $s = \alpha + \beta$, then, the unknown entries of the tridiagonal matrices T_1 and T_2 are given by the following set:

$$\begin{aligned} aa' &= (x - s), \\ a'b^2 - by + av &= 0, \\ b' &= \frac{1}{a}(y - ba'), \\ a'c^2 - cz + aw &= 0, \\ ac' &= (z - ca'). \end{aligned}$$

REMARK. If

$$\Delta_y = y^2 - 4(x-s)v \geq 0,$$
$$\Delta_z = z^2 - 4(x-s)w \geq 0,$$

then T_1 and T_2 are real matrices.

A special case occurs when

$$A = \begin{pmatrix} 1+v & y & v & & & \\ y & 1+2v & . & . & & \\ v & . & . & . & . & \\ & . & . & . & . & v \\ & & . & . & 1+2v & y \\ & & & v & y & 1+v \end{pmatrix} = I + T, \tag{8}$$

where I is the unitary matrix and T is the five-diagonal matrix defined by $T = A - I$. In this case, the set (6) is easily satisfied, $A = T_1T_2$, with

$$T_1 = \mathrm{trid}_n[b,\ 1,\ b], \qquad T_2 = \mathrm{trid}_n\left[b',\ 1,\ b'\right],$$

and

$$b = \frac{y \pm \sqrt{y^2-4v}}{2} \quad \text{and} \quad b' = \frac{y \mp \sqrt{y^2-4v}}{2}. \tag{9}$$

A similar case occurs when

$$A = \begin{pmatrix} 1-v & y & v & & & \\ -y & 1-2v & . & . & & \\ v & . & . & . & . & \\ & . & . & . & . & v \\ & & . & . & 1-2v & y \\ & & & v & -y & 1-v \end{pmatrix} = I + T, \tag{10}$$

for which there exist two Toeplitz matrices

$$T_1 = \mathrm{trid}_n[-b,\ 1,\ b], \qquad T_2 = \mathrm{trid}_n\left[-b',\ 1,\ b'\right], \tag{11}$$

such that $A = T_1T_2$, with b and b' given by (9). We note that, if v is negative, condition $y^2 \geq 4v$ does not impose restriction. If $y^2 \geq 4v$, then T_1 and T_2 are real matrices, while if $y^2 < 4v$, then T_1 and T_2 are complex matrices given by

$$T_1 = \mathrm{Re}(T_1) + i\,\mathrm{Im}(T_1), \qquad T_2 = \mathrm{Re}(T_2) + i\,\mathrm{Im}(T_2),$$

with

$$\mathrm{Re}(T_1) = \mathrm{Re}(T_2), \qquad \mathrm{Im}(T_1) = -\mathrm{Im}(T_2).$$

2. BLOCK FIVE-DIAGONAL MATRICES

Let us consider the class of linear systems (1) in which A is the block five-diagonal matrix of size ns and of the form

$$A = \begin{pmatrix} X-X' & Y & V & & & \\ Z & X & Y & V & & \\ W & Z & X & Y & V & \\ & . & . & . & . & V \\ & & . & . & X & Y \\ & & & W & Z & X-X'' \end{pmatrix}, \tag{12}$$

with X, Y, V, Z, W, X', X'' real matrices of size s. The factorization (4) of A, with T_1 and T_2 block tridiagonal matrices given by

$$T_1 = \mathrm{trid}_{ns}[C, D, B], \qquad T_2 = \mathrm{trid}_{ns}[C', D', B'] \tag{13}$$

holds if and only if the following matrix equations are satisfied:

$$\begin{aligned} DD' + BC' + CB' &= X, \\ DB' + BD' &= Y, \\ DC' + CD' &= Z, \\ BB' &= V, \\ CC' &= W, \\ CB' &= X', \\ BC' &= X''. \end{aligned} \tag{14}$$

If A possesses the following particular form:

$$A = \begin{pmatrix} I+V & Y & V & & & \\ Y & I+2V & \cdot & \cdot & & \\ V & \cdot & \cdot & \cdot & \cdot & \\ & \cdot & \cdot & \cdot & \cdot & V \\ & & \cdot & \cdot & I+2V & Y \\ & & & V & Y & I+V \end{pmatrix} = I + T, \tag{15}$$

the next result holds.

THEOREM 1. *Let $\sqrt{Y^2 - 4V}$, a square root matrix of the nonsingular matrix $Y^2 - 4V$. If Y and $\sqrt{Y^2 - 4V}$ commute, then A in (15) has the factorization $T_1 T_2$ with*

$$T_1 = \mathrm{trid}_{ns}[B, I, B], \qquad T_2 = \mathrm{trid}_{ns}[B', I, B'],$$

and

$$B = \frac{1}{2}\left(Y \pm \sqrt{Y^2 - 4V}\right), \qquad B' = \frac{1}{2}\left(Y \mp \sqrt{Y^2 - 4V}\right).$$

Note that if we consider the square root matrix of $Y^2 - 4V$ that is a polynomial of $Y^2 - 4V$ (see [4]), then, using Theorem 1, it is sufficient that Y and V commute to derive that the factorization (4) holds.

A similar result can be shown when A has a block structure analogous to (10).

3. BOUNDS FOR THE INVERSE

Five-diagonal linear systems are equivalent to discrete boundary value problems with separated boundary conditions. In [5,6], the definition of stability and weak stability for the solution of a discrete BVP have been proposed. The class of boundary value problems (1) (or of linear systems (1)) is said to be *stable*, with respect to the maximum norm $\|\ \|$, if for each n, there exists a unique solution $\mathbf{x}$ and a constant K independent of n such that

$$\|\mathbf{x}\| \le K\|\mathbf{q}\|.$$

While (1) is said to be *weakly stable* if the stability constant K is $O(n^p)$ with $p = 1$ or $p = 2$. For banded linear systems, the study of $\|A^{-1}\|$ is equivalent to that of the stability of the corresponding BVP, and, for Toeplitz matrices, the last is equivalent to find the roots of the polynomial

$$\pi(\lambda) = v\lambda^4 + y\lambda^3 + x\lambda^2 + z\lambda + w$$

associated to A. We will prove that $\|A^{-1}\|$ shows a behaviour, with respect to n, similar to $\|A_T^{-1}\|$, where A_T is the Toeplitz five-diagonal matrix obtained by A replacing the first and the last element of the main diagonal with x. Now we state a known result of the dichotomic theory of discrete BVP, which will be used in Theorem 3 (see [5,6]).

THEOREM 2. *Let T be the real Toeplitz tridiagonal matrix in (3), then the linear system $T\mathbf{x} = \mathbf{q}$ is stable if and only if the associated polynomial*

$$\pi(\lambda) = b\lambda^2 + a\lambda + c$$

possesses one root inside and one root outside the unit circle $B(0,1)$ of the complex plane $\mathbf{C}$, while the linear system is weakly stable if there exists one root on the boundary of $B(0,1)$.

We can show the following result.

THEOREM 3. *Let A be the matrix in (2). Suppose that the factorization $A = T_1T_2$ holds with T_1 and T_2 given by (5), then*

$$\pi(\lambda) = \pi_1(\lambda)\pi_2(\lambda), \tag{16}$$

where $\pi(\lambda)$, $\pi_1(\lambda)$, $\pi_2(\lambda)$ are the polynomial associated to A_T, T_1, T_2, respectively. Moreover, if

$$|b+c| < |a| \quad \textit{and} \quad |b'+c'| < |a'|, \tag{17}$$

then $||A^{-1}|| = O(1)$, while if

$$|b+c| < |a| \quad \textit{and} \quad |b'+c'| = |a'|, \tag{18}$$

then $||A^{-1}|| = O(n^p)$ for $p = 1$ or $p = 2$. Finally, we obtain that $||A^{-1}||$ shows a behaviour similar to $||A_T^{-1}||$.

PROOF. Using (6), then equation (16) may be easily derived. When (17) is verified, both $\pi_1(\lambda)$ and $\pi_2(\lambda)$ have one root inside and one root outside $B(0,1)$. From Theorem 1, it follows that $||{T_1}^{-1}|| = O(1)$, $||{T_2}^{-1}|| = O(1)$, and $||A^{-1}|| = O(1)$ (see [6]). If (18) is verified, then $\pi_1(\lambda)$ has one root inside and one root outside $B(0,1)$ while $\pi_2(\lambda)$ has at least one root on the boundary of $B(0,1)$, thus, from Theorem 1, it follows that $||{T_1}^{-1}|| = O(1)$, $||{T_2}^{-1}|| = O(n^p)$, and hence, $||A^{-1}|| = O(n^p)$ with $p = 1$ or $p = 2$. Finally, since $\pi(z) = \pi_1(z)\pi_2(z)$, it follows that $||{A_T}^{-1}||$ shows a behaviour, with respect to n, similar to $||A^{-1}||$. ∎

For example, if A is given by (8), then $||A^{-1}||$ and $||{A_T}^{-1}||$ are bounded by a constant independent of n because (17) is easily verified.

In the case of block five-diagonal matrices for which (4) holds, bounds for the inverse may be given in terms of $||{T_1}^{-1}||$ and $||{T_2}^{-1}||$. Furthermore, if the blocks C, D, B, and C', D', B', are Teoplitz matrices, then T_1 and T_2 are nearly Teoplitz matrices and a result similar to Theorem 2 may be used in order to bound $||{T_1}^{-1}||$ and $||{T_2}^{-1}||$.

4. SOLUTION OF FIVE-DIAGONAL LINEAR SYSTEMS

In both scalar and block case, the factorization T_1T_2 may be used in place of the standard LU methods based on Gaussian elimination. In fact, if the factorization $A = T_1T_2$ exists with T_1 and T_2 real tridiagonal (or real block tridiagonal) matrices, then the solution of (1) is equivalent to the sequential solution of

$$T_1\mathbf{z} = \mathbf{q}, \qquad T_2\mathbf{x} = \mathbf{z}, \tag{19}$$

where each tridiagonal (or block tridiagonal) system may be solved by a suitable method.

In the scalar case, the cost of the factorization is independent of n, so it may be neglected for large n. Moreover, if we use the LU factorization for both tridiagonal systems in (19), we achieve a sequential method (denoted by sequential T_1T_2 algorithm). This algorithm requires smaller operation than the method based on the LU factorization of the five-diagonal matrix A (the LU five-diagonal algorithm). In fact, $19n - 29$ operations are required by the LU five-diagonal algorithm, and $16n-14$ operations by the sequential T_1T_2 algorithm. Furthermore, we can derive

Table 1. Operation count.

Algorithm	Add	Multiply	Divide	Total
LU	$8n-13$	$8n-13$	$3n-3$	$19n-29$
T_1T_2	$6n-6$	$6n-6$	$4n-2$	$16n-14$
CR	$12k-12$	$16k-16$	$6k-6$	$34k-34$
W	$14k-8$	$18k-12$	$10k-4$	$42k-24$

Table 2. Speed-up.

$\frac{LU}{W}$	$\frac{LU}{CR}$	$\frac{T_1T_2}{W}$	$\frac{T_1T_2}{CR}$
$p\frac{9.5}{21}$	$p\frac{9.5}{17}$	$p\frac{8}{21}$	$p\frac{8}{17}$

a parallel method for solving (1) by the sequential solution of the tridiagonal systems in (19), each one made by a parallel method for tridiagonal systems, for example, Wang algorithm (denoted by W) or the parallel ciclic reduction (denoted by CR) (see [7,8]). In Table 1, we show the number of operations of these algorithms applied to (1). For the parallel algorithms, the number of operations is per processor. The integer k is defined by $n = kp$ where p is the number of processors. The theoretical speed-up, for large n, of Wang and CR algorithm with respect to the LU and T_1T_2 sequential algorithm are given in Table 2. When the factorization $A = T_1T_2$ exists, with T_1 and T_2 complex tridiagonal (or complex block tridiagonal) matrices, then the solution of (19) is equivalent to

$$\begin{aligned} \operatorname{Re}(T_1)\mathbf{z}_1 - \operatorname{Im}(T_1)\mathbf{z}_2 &= \mathbf{q}, \\ \operatorname{Im}(T_1)\mathbf{z}_1 + \operatorname{Re}(T_1)\mathbf{z}_2 &= \mathbf{0}, \end{aligned} \tag{20}$$

and

$$\operatorname{Re}(T_2)\mathbf{x} = \mathbf{z}_1, \qquad (\text{or } \operatorname{Im}(T_2)\mathbf{x} = \mathbf{z}_2), \tag{21}$$

where $\mathbf{z} = \mathbf{z}_1 + i\mathbf{z}_2$. Suppose the preceding system to be equivalent to

$$\begin{aligned} W\mathbf{z}_1 + \mathbf{z}_2 &= c_1\mathbf{q}, \\ -\mathbf{z}_1 + W\mathbf{z}_2 &= c_2\mathbf{q}, \end{aligned} \tag{22}$$

with

$$\mathbf{x} = d_1\mathbf{z}_1 + d_2\mathbf{z}_2, \tag{23}$$

where $W = a_1 \operatorname{Re}(T_1) + a_2 \operatorname{Im}(T_1)$, and $a_1, a_2, d_1, d_2, c_2, c_2$ are suitable constants.

Then, a numerical method for solving (22) may be given by the iterative procedure

$$\begin{aligned} W\mathbf{z}_1^{(m+1)} &= -\mathbf{z}_2^{(m)} + \mathbf{v}_1, \\ W\mathbf{z}_2^{(m+1)} &= \mathbf{z}_1^{(m)} + \mathbf{v}_2, \end{aligned} \tag{24}$$

in which, at each iterate m, we have to solve two independent tridiagonal systems with the same coefficient matrix W.

THEOREM 4. *If $\rho(W^{-1})$ is less than 1, then the iterative method (24) converges.*

PROOF. We observe that the iteration matrix of (24) is given by

$$P = \begin{pmatrix} 0 & -W^{-1} \\ W^{-1} & 0 \end{pmatrix},$$

from which

$$\begin{aligned} \det(\lambda I - P) &= \det \begin{pmatrix} \lambda I & W^{-1} \\ -W^{-1} & \lambda I \end{pmatrix} = \det(\lambda I) \det\left(\lambda I + \left(\frac{1}{\lambda}\right) W^{-1}W^{-1}\right) \\ &= \det\left(\lambda^2 I + W^{-1}W^{-1}\right) = \det\left(\lambda I + iW^{-1}\right)\det\left(\lambda I - iW^{-1}\right). \end{aligned}$$

Thus, the eigenvalues λ of P are $i\nu$ and $-i\nu$, where ν is any eigenvalue of W^{-1}. Then if $\rho(W^{-1}) < 1$, it follows that $|\lambda| < 1$. ∎

However, note that the iterative method (24) will be advantageous on the standard LU five-diagonal algorithms only if the number of iterates required for convergence is small or if a parallel computer is employed for solving simultaneously the couple of tridiagonal systems in (24).

5. APPLICATIONS AND NUMERICAL TESTS

Consider the set of n differential equations of the form

$$\begin{aligned} \mathbf{U}'(t) &= T\mathbf{U}(t) + \mathbf{b}, \\ \mathbf{U}(0) &= \mathbf{g}, \end{aligned} \tag{25}$$

where T is a matrix of size n and $\mathbf{b}$ a known vector. The solution of (25) may be written as

$$\mathbf{U}(t+k) = \exp(kT)\left(\mathbf{U}(t) - T^{-1}\mathbf{b}\right) + T^{-1}\mathbf{b}, \tag{26}$$

where $k > 0$ denotes the time step. Thus, by using an approximation of the exponential matrix $\exp(kT)$, we can derive a numerical method providing an approximation $\mathbf{v}(t+k)$ of $\mathbf{U}$ at $t+k$. Common implicit numerical methods derive from the use of the general (r,s)-Padè approximation for $r \geq 1$ of the exponential $\exp(kT)$ in (26) (see, for example, [9]). If the matrix T in (26) has the form (8), then the $(1,s)$-Padè approximations of the exponential $\exp(kT)$ for $s = 0, 1$, require the inverse a five-diagonal matrix.

COROLLARY 1. *If the matrix T in (25) is the five-diagonal matrix T defined in (8) or in (10), then the factorization T_1T_2 holds for both $(I - kT)$ and $(I - (1/2)kT)$. If $v > 0$, then T_1 and T_2 are real matrices.*

COROLLARY 2. *Let T be a Toeplitz tridiagonal matrix. Consider $[Q_2^s(kT)]^{-1}P_s^2(kT)$, the (2,s)-Padè approximations of $\exp(kT)$, for $s = 0,1,2$. Then $[Q_2^s(kT)]$, for $s = 0,1,2$, are five-diagonal matrices of the form (2) for which the factorization T_1T_2 exists with T_1 and T_2 complex tridiagonal matrices.*

PROOF. For simplicity, assume $k = 1$. Consider the $(2,s)$-Padè approximations of $\exp(T)$ for $s = 0,1,2$, respectively, given by

$$\begin{aligned} \exp(T) &\simeq \left[Q_2^0(T)\right]^{-1} P_0^2(T) = \left(I - T + \frac{1}{2}T^2\right)^{-1}, \\ \exp(T) &\simeq \left[Q_2^1(T)\right]^{-1} P_1^2(T) = \left(I - \frac{2}{3}T + \frac{1}{6}T^2\right)^{-1}\left(I + \frac{1}{3}T\right), \\ \exp(T) &\simeq \left[Q_2^2(T)\right]^{-1} P_2^2(T) = \left(I - \frac{1}{2}T + \frac{1}{12}T^2\right)^{-1}\left(I + \frac{1}{2}T + \frac{1}{12}T^2\right), \end{aligned}$$

and observe that the thesis follows from the known result that the polynomials $Q_2^s(z)$, for $s = 0,1,2$, are of degree 2 with complex roots. ∎

Similar results may be shown in the case of block tridiagonal matrices. As numerical test, we consider the constant coefficient heat equation in one space variable

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial^2 u}{\partial x^2}x, && \in [0,\pi], \qquad t \geq 0, \\ u(x,0) &= \sin x, && x \in [0,\pi], \\ u(0,t) &= u(\pi,t) = 0, && t \geq 0, \end{aligned} \tag{27}$$

the theoretical solution of which is $u(x,t) = \exp(-t)\sin x$. Let $h = \pi/(n+1)$ with n positive integer and approximate $u(mh,t)$ by $U_m(t)$ for $m = 0, 1, \dots, n+1$, with $U_0(t) = U_{n+1}(t) = 0$. Using second-order finite-difference to approximate partial derivatives with respect to x, it follows that $\mathbf{U}(t) = (U_1(t), \dots, U_n(t))^\top$ satisfies (25) where $\mathbf{g} = (g(h), \dots, g(nh))^\top$, $\mathbf{b} = 0$, and $T = (1/h^2)\mathrm{trid}_n[1,\ -2,\ 1]$. The implicit numerical algorithm derived by the $(2,0)$-Padè approximation of $\exp(kT)$ leads to the numerical solution of the linear systems

$$A\mathbf{v}(t+k) = \mathbf{v}(t), \qquad t = 0, k, 2k, \dots, \tag{28}$$

where A is a symmetric five-diagonal matrix for which, due to Corollary 2, a complex factorization T_1T_2 exists. In particular, we have

$$A = \frac{1}{2}[(1+i)I - kT][(1-i)I - kT]. \tag{29}$$

The complex linear system (28) may be written in the form (22),(23), in particular, we have

$$\begin{aligned} (I - kT)\mathbf{z}_1 - \mathbf{z}_2 &= 2\mathbf{v}(t), \\ \mathbf{z}_1 + (I - kT)\mathbf{z}_2 &= 0, \end{aligned} \tag{30}$$

the solution of which is $\mathbf{v}(t+k) = -\mathbf{z}_2$, while the iterative method (24) becomes

$$\begin{aligned} (I - kT)\mathbf{z}_1^{(m+1)} &= \mathbf{z}_2{}^{(m)} + 2\mathbf{v}(t), \\ (I - kT)\mathbf{z}_2^{(m+1)} &= -\mathbf{z}_1^{(m)}, \end{aligned} \tag{31}$$

which converges since the eigenvalues of the matrix $(I - kT)$ have modulus greater than 1. For solving each linear system in (31), we have used the LU five-diagonal algorithm and the iterative method (31) with initial vector $\mathbf{z}_2^{(0)} = -\mathbf{v}(t)$ and $\mathbf{z}_1^{(0)} = \mathbf{v}(t)$. We have iterated (31) until the global error, at the time fixed, has been of the same magnitude of that obtained by the LU algorithm. We have achieved that, after a small time interval, a very small number of iterations is required for the convergence. Thus, at least after this initial time interval, the numerical method based on the iterative procedure (31) seems to be more efficient based on the direct method. In Table 3, we compare the CPU times in sec of the two methods applied on the whole time interval $[0, 15]$. These numerical results have been obtained using a Matlab code on a computer Alpha 200 4/233.

Table 3.

	Method (28)	LU Algorithm
h	CPU	CPU
$\frac{\pi}{200}$	7.68	6.6
$\frac{\pi}{400}$	16.01	15.35
$\frac{\pi}{800}$	34.23	39.63
$\frac{\pi}{1600}$	84.33	118.38
$\frac{\pi}{3200}$	289.71	372.73

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