Abstract The solution of certain Toeplitz linear systems is considered in this paper. This kind of systems are encountered when we solve certain partial differential equations by finite difference techniques and approximate functions using higher order splines. The methods presented here are more efficient than the Cholesky decomposition method and are based on the circulant factorization of the "banded circulant" matrix, the use of the Woodbury formula and algebraic perturbation method.

On The Solution of A Class of Toeplitz Systems

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1. Introduction

We wish to consider the linear system of the form

$$Ax = f, \tag{1.1}$$

where the coefficient matrix is an nth order symmetric banded matrix of Toeplitz form

$$A_t = \begin{pmatrix}
a_0 & a_1 & \cdots & a_p & & & & & & \\
a_1 & \ddots & \ddots & & \ddots & & & & & \\
\vdots & \ddots & \ddots & \ddots & & \ddots & & & & \\
a_p & & \ddots & \ddots & \ddots & & \ddots & & & \\
 & \ddots & & \ddots & \ddots & \ddots & & \ddots & & \\
 & & \ddots & & \ddots & \ddots & \ddots & & \ddots & \\
 & & & \ddots & & \ddots & \ddots & \ddots & & a_p \\
 & & & & \ddots & & \ddots & \ddots & \ddots & \vdots \\
 & & & & & \ddots & & \ddots & \ddots & a_1 \\
 & & & & & & a_p & \cdots & a_1 & a_0
\end{pmatrix}, \tag{1.2}$$

or cyclic form

$$A_c = \begin{pmatrix}
a_0 & a_1 & \cdots & a_p & & & & a_p & \cdots & a_1 \\
a_1 & \ddots & \ddots & & \ddots & & & & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & & \ddots & & & & a_p \\
a_p & & \ddots & \ddots & \ddots & & \ddots & & & \\
 & \ddots & & \ddots & \ddots & \ddots & & \ddots & & \\
 & & \ddots & & \ddots & \ddots & \ddots & & \ddots & \\
 & & & \ddots & & \ddots & \ddots & \ddots & & a_p \\
a_p & & & & \ddots & & \ddots & \ddots & \ddots & \vdots \\
\vdots & \ddots & & & & \ddots & & \ddots & \ddots & a_1 \\
a_1 & \cdots & a_p & & & & a_p & \cdots & a_1 & a_0
\end{pmatrix}, \tag{1.3}$$

$x = (x_1, x_2, \ldots, x_n)^T$ is the unknown n-vector, and f is the given right hand side.

This class of linear systems occures in solving certain kind of boundary value problems by finite difference techniques, solving biharmonic equation by Fourier method, and in higher order spline approximation[2, 3, 4, 6, 10].

System (1.1) with coefficient matrix of form (1.2) can be solved by band Cholesky decomposition[7] or by Toeplitz factorization[6]. Although the operation counts of the two methods are about the same the later one requires less storages. If the system has coefficient matrix of form (1.3), then the Cholesky decomposition is expensive, and the circulant factorization presented here is more favorable in terms of not only arithmetic operations but also storage requirements. The methods presented in this paper are based on the fact that under certain condition the matrix in (1.3) can be factored into two simpler circulant matrices, and the corresponding circulant system may then be solved by using the Woodbury formula[8]. Furthermore, the banded Toeplitz matrix may be treated as a perturbation of circulant matrix, and Toeplitz systems can be solved by the combination of the circulant factorization and the use of algebraic perturbation method[9].

In §2, we will describe the method for factoring a symmetric banded circulant matrix into two circulant matrices, and then use the factors to solve the band circulant system in §3. The methods for solving band Toeplitz systems will be studied in §4, and finally, some numerical results will be given in §5.

2. Factorization of banded Circulant Matrices

To factor the banded circulant matrix given by (1.3) we consider the real polynomial with the elements of the matrix as its coefficients

$$\phi(z) = a_p z^p + \cdots + a_1 z + a_0 + a_1 z^{-1} + \cdots + a_p z^{-p}, \tag{2.1}$$

the characteristic function of matrix A. Assume, without loss of generality, that $a_p = 1$. We have the following theorem.

Theorem 2.1. *If matrix A is strictly diagonal dominant, i.e. $|a_0| > 2(|a_1| + \cdots + |a_p|)$, then there exists a real polynomial $l(z) = \beta_0 + \beta_1 z + \cdots + \beta_p z^p$, $|\beta_0| > 1$, $\beta_p = 1$, with all roots outside the unit circle such that the characteristic function $\phi(z)$ can be factored as*

$$\phi(z) = \frac{1}{\beta_0} l(z) \cdot l(z^{-1}). \tag{2.2}$$

Proof. We show at first that the polynomial $\phi(z)$ has no root on the unit circle. If there exists a number z_0 on the unit circle which is a root of the equation

$$\phi(z) = 0, \tag{2.3}$$

then $z_0 = e^{i\theta}$ for some real θ, $0 \le \theta < 2\pi$. Substituting z_0 into (2.3) we have

$$\begin{aligned} a_0 &= -\left[a_1\left(e^{i\theta} + e^{-i\theta}\right) + \cdots + a_p\left(e^{ip\theta} + e^{-ip\theta}\right)\right] \\ &= -2\left[a_1 \cos\theta + \cdots + a_p \cos p\theta\right]. \end{aligned}$$

It follows that

$$|a_0| \le 2(|a_1| + \cdots + |a_p|),$$

which is a contradiction to the assumption of the theorem.

We now note that

$$\phi(z) = \phi(z^{-1}),$$

and (2.3) is a reciprocal equation[1]. Thus if z_0 is a root of (2.3), then so is z_0^{-1}. It follows that $\phi(z)$ has p pairs of roots $z_1^{(k)}$, $z_2^{(k)}$, such that

$$z_1^{(k)} = \frac{1}{z_2^{(k)}}, \qquad k = 1, 2, \ldots, p,$$

and $z_1^{(k)}$ are outside the unit circle.

Let

$$l(z) = \prod_{k=1}^{p} \left(z - z_1^{(k)}\right). \tag{2.4}$$

We now prove that $l(z)$ is a real polynomial. If all the roots $z_1^{(k)}$ are real, then $p(z)$ is real; if some of the $z_1^{(k)}$'s are complex, then their conjugate complex numbers, which are outside the unit circle too, are the roots of (2.3) since the coefficients of the equation are real. So, it is obvious that $l(z)$ is a real polynomial and satisfies (2.2), and the proof is completed.

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It is easy to verify that the corresponding circulant matrix A_c can be factored as

$$A_c = \beta_0^{-1} \tilde{L} \tilde{L}^T, \tag{2.5}$$

where

$$\tilde{L} = \begin{pmatrix} \beta_0 & & & & \beta_p & \cdots & \beta_1 \\ \vdots & \ddots & & & & \ddots & \vdots \\ \beta_p & & \ddots & & & & \beta_p \\ & \ddots & & \ddots & & & \\ & & \ddots & & \ddots & & \\ & & & \ddots & & \ddots & \\ & & & & \beta_p & \cdots & \beta_0 \end{pmatrix}.$$

To compute the factor $l(z)$, we solve the equation (2.3). When $p = 2$ it is well known[1, 5] that the roots of equation (2.3) are given by

$$(2.6)\qquad \begin{cases} \rho_1 = \frac{1}{2}\left[\eta_1 + \sqrt{\eta_1^2 - 4}\right], \\ \rho_2 = \frac{1}{2}\left[\eta_1 - \sqrt{\eta_1^2 - 4}\right], \\ \rho_3 = \frac{1}{2}\left[\eta_2 + \sqrt{\eta_2^2 - 4}\right], \\ \rho_4 = \frac{1}{2}\left[\eta_2 - \sqrt{\eta_2^2 - 4}\right], \end{cases}$$

where

$$(2.7)\qquad \begin{cases} \eta_1 = \frac{1}{2}\left[-a_1 + \sqrt{a_1^2 - 4a_0 + 8}\right], \\ \eta_2 = \frac{1}{2}\left[-a_1 - \sqrt{a_1^2 - 4a_0 + 8}\right]. \end{cases}$$

Having computed the roots we choose the two roots the absolute values of which are greater than 1 as $z_1^{(1)}$ and $z_1^{(2)}$, and form the coefficients of the factor $l(z)$ via

$$(2.8)\qquad \begin{cases} \beta_0 = z_1^{(1)} z_1^{(2)}, \\ \beta_1 = -\left(z_1^{(1)} + z_1^{(2)}\right), \\ \beta_2 = 1. \end{cases}$$

When p is greater than 2 we have to use some numerical method, for example the Newton-Raphson method, to solve equation (2.3), and then use the relations between the roots and coefficients to calculate the factor $l(z)$.

3. The Solution of Band Circulant Systems

In this section we will use the circulant factorization described in the previous section to develop a method for solving the band circulant system

$$(3.1)\qquad A_c x = f$$

as well as computing the inverse of banded circulant matrices.

It is evident that the system can be solved by solving following two systems

$$(3.2)\qquad \widetilde{L} y = d$$

and

$$\widetilde{L}^T x = y, \tag{3.3}$$

where

$$d = \beta_0 f. \tag{3.4}$$

Let

$$L = \begin{pmatrix} \beta_0 & & & & \\ \vdots & \ddots & & & \\ \beta_p & & \ddots & & \\ & \ddots & & \ddots & \\ & & \ddots & & \ddots & \\ & & & \beta_p & \cdots & \beta_0 \end{pmatrix},$$

and

$$R = \begin{pmatrix} \beta_p & \cdots & \beta_1 \\ & \ddots & \vdots \\ & & \beta_p \end{pmatrix}.$$

Then $\widetilde{L}$ can be written

$$\widetilde{L} = L + \begin{pmatrix} I_p \\ O \end{pmatrix} R (O^T \quad I_p),$$

where I_p is the pth order identity matrix and O the $(n-p)$-by-p zero matrix. Using the Woodbury formula[8], the inverse is given by

$$\widetilde{L}^{-1} = L^{-1} - L^{-1} \begin{pmatrix} I_p \\ O \end{pmatrix} \left[R^{-1} + (O^T \quad I_p) L^{-1} \begin{pmatrix} I_p \\ O \end{pmatrix} \right]^{-1} (O^T \quad I_p) L^{-1},$$

and the solution of (3.2) is

$$y = L^{-1} d - L^{-1} \begin{pmatrix} I_p \\ O \end{pmatrix} \left[R^{-1} + (O^T \quad I_p) L^{-1} \begin{pmatrix} I_p \\ O \end{pmatrix} \right]^{-1} (O^T \quad I_p) L^{-1} d,$$

or

$$y = h - Wg, \tag{3.5}$$

where $h = (h_1, h_2, \ldots, h_n)^T$, W and g are the solution of the following equations, respectively

$$Lh = d, \tag{3.6}$$

$$LW = \begin{pmatrix} I_p \\ O \end{pmatrix}, \tag{3.7}$$

$$Bg = z, \tag{3.8}$$

and

$$z = \begin{pmatrix} h_{n-p+1} \\ \vdots \\ h_n \end{pmatrix},$$

$$B = R^{-1} + (O^T \quad I_p)L^{-1}\begin{pmatrix} I_p \\ O \end{pmatrix}. \tag{3.9}$$

To compute the pth order matrix B, we first solve the equation (3.7). Since W is the first p columns of L^{-1}, and L is a lower triangular Toeplitz matrix and so is its inverse, W is uniquely defined by the first column of L^{-1}, which is the solution of the equation

$$Lw = (1,0,\ldots,0)^T, \tag{3.10}$$

and can be computed with $O(pn)$ operations.

Denote by $w_1, w_2, \ldots, w_n$ the components of vector w, then we have

$$W = \begin{pmatrix} w_1 & & & \\ w_2 & w_1 & & \\ \vdots & \vdots & \ddots & \\ \vdots & \vdots & & w_1 \\ \vdots & \vdots & & \vdots \\ w_n & w_{n-1} & \cdots & w_{n-p+1} \end{pmatrix}, \tag{3.11}$$

and

$$(O^T \quad I_p)W = \begin{pmatrix} w_{n-p+1} & w_{n-p} & \cdots & w_{n-2p+2} \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \\ w_n & w_{n-1} & \cdots & w_{n-p+1} \end{pmatrix}, \tag{3.12}$$

which is also a Toeplitz matrix.

The matrix R^{-1} is an upper triangular Toeplitz matrix and can be calculated with $O(p^2)$ operations. Thus B is Toeplitz, so solving (3.8) will cost $O(p^2)$ operations. Having computed B

and solved the equations (3.6), (3.7) and (3.8), the auxiliary vector y can be found, and we can then solve equation (3.3) in a similar way. Since

$$\tilde{L}^{-T} = L^{-T} - L^{-T}\begin{pmatrix} O \\ I_p \end{pmatrix} B^{-T}(\, I_p \quad O^T\,)L^{-T},$$

and

$$x = L^{-T}y - L^{-T}\begin{pmatrix} O \\ I_p \end{pmatrix} B^{-T}(\, I_p \quad O^T\,)L^{-T}y,$$

the solution vector x is given by

$$x = r - Vs, \tag{3.13}$$

where $r = (r_1, r_2, \ldots, r_n)^T$ is the solution of the equation

$$L^T r = y, \tag{3.14}$$

and

$$V = \begin{pmatrix} w_{n-p+1} & w_{n-p+2} & \cdots & w_n \\ w_{n-p} & w_{n-p+1} & \cdots & w_{n-1} \\ \vdots & \vdots & & \vdots \\ w_1 & w_2 & \cdots & w_{n-p+1} \\ & w_1 & & \vdots \\ & & \ddots & \vdots \\ & & & w_1 \end{pmatrix}, \tag{3.15}$$

and s is the solution of the equation

$$B^T s = (r_1, r_2, \ldots, r_p)^T. \tag{3.16}$$

The asymptotic operation counts of the method would be $O(5pn)$ excluding the amount of work to calculate the factor $l(z)$. In most usual case, $p = 1$ or 2, and finding $l(z)$ does not cost much work. The algorithm may be summarized as follows.

Algorithm BCS (Banded Circulant Solver) solves banded circulant system (3.1). Assume that the parameters β_0, β_1, ..., β_p are precomputed.

1. Solve equation (3.6) for h by forward substitution.
2. Solve equation (3.10) and form W via (3.11).

3. Compute R^{-1} by backward substitution, and form matrix B.

4. Solve equation (3.8) for g using a Toeplitz type method.

5. Calculate the solution vector y of (3.2) via (3.5).

6. Solve equation (3.14) for r.

7. Form V via (3.15).

8. Solve (3.16) for s.

9. Compute the solution vector x via (3.13).

endalgorithm

Algorithm BCS can be modified to compute the inverse of banded circulant matrix. Since A_c is a symmetric circulant matrix its inverse A_c^{-1} is also a symmetric circulant, which is uniquely defined by its first column, that is the solution of the equation

$$A_c u = (1, 0, \ldots, 0)^T. \tag{3.17}$$

The algorithm BCS may directly be employed to solve equation (3.17). But in this case the first two steps of the algorithm are essentially the same, so we obtain the following algorithm for inverting banded circulant matrix requiring $O(4pn)$ operations by modifying the first two steps of the algorithm BCS and computing the solution of equation

$$\widetilde{L} y = \beta_0 (1, 0, \ldots, 0)^T, \tag{3.18}$$

instead of equation (3.2) in step 5 of the algorithm BCS.

Algorithm BCI (Banded Circulant Inverse) computes the inverse of banded circulant matrix. Assume that the parameters β_0, β_1, ..., β_p are precomputed.

1. Solve equation (3.10) and form W via (3.11).

2. Compute $h = \beta_0 w$.

3. Compute R^{-1} by backward substitution, and form matrix B.

4. Solve equation (3.8) for g using a Toeplitz type method.

5. Calculate the solution vector y of (3.18).

6. Solve equation (3.14) for r.

7. Form V via (3.15).

8. Solve (3.16) for s.

9. Compute the first column of the desired inverse via (3.13) and form it.

endalgorithm

4. Band Toeplitz Systems

The band Cholesky decomposition is an efficient method for solving general band symmetric systems[7], and it can of cource be used to solve band Toeplitz system

$$A_t x = f. \tag{4.1}$$

But the application of this method to Toeplitz systems not only costs a lot of arithmetic operations but also requires a great amount of storages since it does not take the advantage of the structure of Toeplitz matrix. Fischer etc.[6] proposed the Toeplitz factorization method for the solution of band Toeplitz systems, which has some advantages both in terms of arithmetic operations and storage requirements. In this section we will use the circulant method described in last section to develop an alternative to the Toeplitz factorization for solving band Toeplitz system (4.1).

Banded Toeplitz matrix A_t may be considered to be a $(2p)$-rank perturbation of the banded circulant matrix A_c, i.e.

$$A_t = A_c - \begin{pmatrix} I_p \\ O \end{pmatrix} U (O^T \quad I_p) - \begin{pmatrix} O \\ I_p \end{pmatrix} U^T (I_p \quad O^T). \tag{4.2}$$

where

$$U = \begin{pmatrix} a_p & \cdots & a_1 \\ & \ddots & \vdots \\ & & a_p \end{pmatrix}.$$

Substituting (4.2) into (4.1) we have

$$A_c x - \begin{pmatrix} I_p \\ O \end{pmatrix} U (O^T \quad I_p) x - \begin{pmatrix} O \\ I_p \end{pmatrix} U^T (I_p \quad O^T) x = f. \tag{4.3}$$

If matrix A_t is strictly diagonal dominant, then the corresponding circulant matrix A_c is likewise, and therefore is nonsingular, and from (4.3) we have

$$x - A_c^{-1} \begin{pmatrix} I_p \\ O \end{pmatrix} U (O^T \quad I_p) x - A_c^{-1} \begin{pmatrix} O \\ I_p \end{pmatrix} U^T (I_p \quad O^T) x = A_c^{-1} f. \tag{4.4}$$

Let $x^{(1)} = (x_1, \ldots, x_p)^T$, $x^{(2)} = (x_{p+1}, \ldots, x_{n-p})^T$, and $x^{(3)} = (x_{n-p+1}, \ldots, x_n)^T$, and

$$B_1 = A_c^{-1} \begin{pmatrix} I_p \\ O \end{pmatrix},$$

$$B_3 = A_c^{-1}\begin{pmatrix} O \\ I_p \end{pmatrix},$$

which are the n-by-p submatrices consisting of the first and the last p columns of matrix A_c^{-1}, respectively. Then equation (4.4) becomes

$$x = y + B_1 U x^{(3)} + B_3 U^T x^{(1)}, \tag{4.5}$$

which shows that the solution to equation (4.1) is the linear combination of the solution of the corresponding circulant system

$$A_c y = f \tag{4.6}$$

and the first p and the last p columns of the inverse of the corresponding circulant matrix.

The solution to (4.6) can be obtained by algorithm BCS in $O(5pn)$ operations, and the inverse of A_c can be calculated in $O(4pn)$ operations by using algorithm BCI. The inverse A_c^{-1} is, as we pointed out above, symmetric circulant and defined by its first column, the elements of which are denoted by $u_1, u_2, \ldots, u_n$ satisfying

$$u_{n-i} = u_{i+2}, \qquad i = 0, 1, \ldots, \lfloor (n-2)/2 \rfloor,$$

where $\lfloor z \rfloor$ is the integer floor function of z. We then have

$$A_c^{-1} = \begin{pmatrix} u_1 & u_2 & \cdots & \cdots & u_n \\ u_2 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & u_2 \\ u_n & \cdots & \cdots & u_2 & u_1 \end{pmatrix},$$

and therefore

$$B_1 = \begin{pmatrix} u_1 & \cdots & \cdots & u_p \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \vdots & & & u_1 \\ u_{n-p+1} & & & \vdots \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ u_n & \cdots & \cdots & u_{n-p+1} \end{pmatrix}, \tag{4.7}$$

and

$$(4.8) \qquad B_3 = \begin{pmatrix} u_{n-p+1} & \cdots & \cdots & u_n \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \vdots & & & u_{n-p+1} \\ u_1 & & & \vdots \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ u_p & \cdots & \cdots & u_1 \end{pmatrix}.$$

To compute the first p and the last p components of the unknown vector x, we premultiply equation (4.5) by $(\, I_p \quad O^T \,)$ and $(\, O^T \quad I_p \,)$, respectively, resulting the following linear system

$$(4.9) \qquad \begin{cases} \left(I_p - M_{1p}U^T\right) x^{(1)} - M_{11}Ux^{(3)} = y^{(1)}, \\ -M_{11}U^T x^{(1)} + \left(I_p - M_{1p}^T U\right) x^{(3)} = y^{(3)}, \end{cases}$$

where M_{11} and M_{1p} are the pth order submatrices of A_c^{-1} at the northwest and northeast corner, respectively, i.e.

$$M_{11} = \begin{pmatrix} u_1 & \cdots & \cdots & u_p \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ u_p & \cdots & \cdots & u_1 \end{pmatrix},$$

$$M_{1p} = \begin{pmatrix} u_{n-p+1} & \cdots & \cdots & u_n \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ u_{n-2p+2} & \cdots & \cdots & u_{n-p+1} \end{pmatrix},$$

and $y^{(1)}$, $y^{(3)}$ are the p-vectors with the first and the last p components of vector y as their elements, respectively.

Forming the coefficients of equation (4.9) will cost $O(2p^2)$ operations and (4.9) can be solved by Gaussian elimination with $O(8p^3)$ operations. Having calculated y, u, $x^{(1)}$ and $x^{(3)}$, the subvector $x^{(2)}$ can be obtained via (4.5) with $O(2pn)$ operations. When $p \ll n$, the asymptotic operation counts of the algorithm would be $O(11pn)$ excluding the amount of work to compute the factor $l(z)$. The algorithm thus procceds as follows.

Algorithm BTS (Band Toeplitz Solver) solves band Toeplitz system (4.1). Assume that the parameters β_0, β_1, ..., β_p are precomputed.

1. Solve for y equation (4.6) by using algorithm BCS.
2. Compute the first column vector u of A_c^{-1} using algorithm BCI.
3. Form and solve equation (4.9) for $x^{(1)}$ and $x^{(3)}$.
4. Compute vector $x^{(2)}$ via (4.5), which along with $x^{(1)}$ and $x^{(3)}$ is the solution.

endalgorithm

5. Numerical Experiments

The algorithms described in this paper were tried on the APVAX of the Department of Computer Science, Yale University, and compared with Toeplitz factorization and Cholesky decomposition. The programs were written and timed in FORTRAN.

To obtain some insight of the accuracy of the algorithms, we generated a number of vectors randomly, which were considered to be the "exact" solutions and then multiplied them by the coefficient matrices to generate the corresponding right hand sides. The equations were solved by using the algorithm BCS and BTS as well as the Toeplitz factorization and Cholesky method. In all the experiments the results differ from the "exact" solutions only in the last digit, indicating that the algorithms presented in this paper are stable.

In our all tests we let $p = 2$ and chose several matrices satisfying the assumption in theorem 2.1. The execution time of algorithm BTS and the Toeplitz factorization are almost the same. For solving circulant systems the algorithm BCS is about twenty times faster than the Cholesky method in our tests, and saves a lot of storages.

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