Inversion of Toeplitz Band Matrices

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Abstract. An algorithm for inverting Toeplitz matrices is simplified for Toeplitz band matrices. In some cases, the simplification yields formulas for the elements in the first row and column of the inverse, from which the remaining elements can be easily calculated. Two examples are given. In any case, the simplification yields a recursive method for computing the first row and column of the inverse of an nth order Toeplitz band matrix with $O(n)$ operations, where $O(n^2)$ are required with the more general algorithm.

1. **Introduction.** A Toeplitz matrix is of the form

$$(1) \qquad T_n = \begin{bmatrix} \phi_0 & \phi_{-1} & \phi_{-2} & \cdots & \phi_{-n} \\ \phi_1 & \phi_0 & \phi_{-1} & \cdots & \phi_{-n+1} \\ & & \cdots & & \\ \phi_n & \phi_{n-1} & \phi_{n-2} & \cdots & \phi_0 \end{bmatrix} = [\phi_{r-s}]_{r,s=0}^n.$$

In [5], the author derived an algorithm for inverting a hermitian Toeplitz matrix T_n with $O(n^2)$ operations (rather than $O(n^3)$, as required by standard matrix inversion methods) and stated a similar algorithm for the nonhermitian case. These algorithms require that all principal minors of T_n be nonzero. Zohar [8] derived the extended algorithm in detail, and Akaike [1] generalized Zohar's derivation to block Toeplitz matrices. Bareiss [2] gave an algorithm for solving the linear system $T_n x = y$ with $O(n^2)$ operations.

In this paper, we simplify the more general algorithm of [5] for the case where T_n is a Toeplitz *band* matrix, by which we mean that there are integers p and q, $1 \leqslant p, q < n$, such that

$$(2) \qquad \phi_p \neq 0, \quad \phi_{-q} \neq 0, \quad \phi_r = 0 \quad \text{if } r > p \text{ or } r < -q.$$

In some cases, including two recently treated by quite different methods [3], [4], this simplification yields formulas for the elements of the first row and column of T_n^{-1}, from which its remaining elements can easily be calculated by Theorem 1, below. In any case, the simplification yields the first row and column of T_n^{-1} with $O(n)$ operations, where $O(n^2)$ operations are required for the more general procedure of [5].

2. **Computation of** T_n^{-1} **from its First Row and Column.** We follow the notation of [5]; therefore, in applying the results given here, the reader should note that T_n is of order $n + 1$. If T_{n-1} is nonsingular, we define $\{\psi_{0,n-1}, \cdots, \psi_{n-1,n-1}\}$ and $\{\eta_{0,n-1}, \cdots, \eta_{n-1,n-1}\}$ by

$$(3) \qquad \sum_{s=0}^{n-1} \phi_{r-s}\,\psi_{s,n-1} = \phi_{r+1}, \qquad 0 \leqslant r \leqslant n-1,$$

and

$$(4) \qquad \sum_{s=0}^{n-1} \phi_{s-r}\,\eta_{s,n-1} = \phi_{-r-1}, \qquad 0 \leqslant r \leqslant n-1.$$

We state the following theorem for reference below.

THEOREM 1. *If* T_n *and* T_{n-1} *are both nonsingular, then* $T_n^{-1} = [b_{rsn}]_{r,s=0}^{n}$ *is given by*

$$(5) \qquad b_{00n} = \Delta_{n-1}^{-1};$$

$$(6) \qquad b_{r0n} = -\Delta_{n-1}^{-1}\,\psi_{r-1,n-1}, \qquad 1 \leqslant r \leqslant n;$$

$$(7) \qquad b_{0sn} = -\Delta_{n-1}^{-1}\,\eta_{s-1,n-1}, \qquad 1 \leqslant s \leqslant n;$$

and

$$(8) \qquad b_{rsn} = b_{r-1,s-1,n} + \Delta_{n-1}^{-1}(\psi_{r-1,n-1}\,\eta_{s-1,n-1} - \eta_{n-r,n-1}\,\psi_{n-s,n-1}),$$
$$1 \leqslant r,\ s \leqslant n,$$

where

$$(9) \qquad \Delta_{n-1} = \phi_0 - \sum_{s=0}^{n-1} \phi_{s+1}\,\eta_{s,n-1}$$

or, equivalently,

$$(10) \qquad \Delta_{n-1} = \phi_0 - \sum_{s=0}^{n-1} \phi_{-s-1}\,\psi_{s,n-1}.$$

Equations (5)–(8) are stated in [5], but derived there only for hermitian T_n. The derivation for the general case appears in [8]. Equations (9) and (10) do not appear in [5] or [8], but the special case to which they both reduce when T_n is hermitian is derived in [5]; the same proof yields (9) and (10).

3. **The Difference Equations.** Theorem 1 says that if T_n and T_{n-1} are nonsingular, then T_n^{-1} can easily be calculated from the solutions of (3) and (4). The following theorem shows that if T_n is a band matrix, these solutions can be found by solving two difference equations of order $p + q$.

THEOREM 2. *If* T_{n-1} *is nonsingular and* $\{\phi_j\}$ *satisfies* (2), *then* $\{\psi_{j,n-1}\}_{j=0}^{n-1}$ *can be extended to all integers* j *as the solution of the difference equation*

$$(11) \qquad \sum_{i=-q}^{p} \phi_i\,\psi_{r-i,n-1} = 0, \qquad -\infty < r < \infty,$$

that satisfies the conditions

(12)
$$\psi_{j,n-1} = 0, \qquad n \leqslant j \leqslant n + q - 1,$$
$$\psi_{j,n-1} = -\delta_{-1,j}, \qquad -p \leqslant j \leqslant -1.$$

Similarly, $\{\eta_{j,n-1}\}_{j=0}^{n-1}$ *can be extended to all* j *as the solution of*

(13)
$$\sum_{i=-q}^{p} \phi_i \eta_{r+i,n-1} = 0, \qquad -\infty < r < \infty,$$

that satisfies

(14)
$$\eta_{j,n-1} = 0, \qquad n \leqslant j \leqslant n + p - 1,$$
$$\eta_{j,n-1} = -\delta_{-1,j}, \qquad -q \leqslant j \leqslant -1.$$

In terms of these extended sequences, (9) *and* (10) *can be rewritten as*

(15)
$$\Delta_{n-1} = \phi_{-q} \eta_{-q-1,n-1}$$

and

$$\Delta_{n-1} = \phi_p \psi_{-p-1,n-1}.$$

We omit the routine verification of this theorem. A special case, applicable to hermitian T_n, has been stated and used [6], [7] for finding minimum variance prediction formulas for finite moving-average processes.

Example 1. Hoskins and Ponzo [3] have given formulas for the inverses of Toeplitz band matrices with

(16)
$$\phi_j = (-1)^j \binom{k}{m+j},$$

in the case where $k = 2r$ and $m = r$. Theorems 1 and 2 yield T_n^{-1} when k and m are any integers such that $1 \leqslant m \leqslant k - 1$.

Let $p = k - m$ and $q = m$ in Theorem 2. With ϕ_j as defined by (16), the solutions of (11) and (13) are polynomials of degree not exceeding $k - 1$. Applying (12) and (14) yields

(17)
$$\psi_{j,n-1} = \frac{(-1)^{m-1}(j-n-m+1)_m (j+2)_{k-m-1}}{(n+1)_m (k-m-1)!}$$

and

(18)
$$\eta_{j,n-1} = \frac{(-1)^{k-m-1}(j-n-k+m+1)_{k-m}(j+2)_{m-1}}{(n+1)_{k-m}(m-1)!},$$

where
$$(x)_0 = 1, \quad (x)_s = x(x+1)\cdots(x+s-1), \quad s \geqslant 1.$$

Equation (15) yields

(19)
$$\Delta_{n-1} = (n+m+1)_{k-m}/(n+1)_{k-m}.$$

Given (17), (18) and (19), T_n^{-1} can now be obtained from (5)–(8).

Example 2. Rehnqvist [4] has given a method for inverting Toeplitz band matrices with

(20)
$$\phi_j = 1 - |j|/m \quad \text{if } |j| < m,$$
$$= 0 \quad\quad\quad \text{if } |j| \geqslant m.$$

If
$$x_r = \frac{1}{\sqrt{m}} \sum_{j=1}^{m} y_{j+r}, \quad -\infty < r < \infty,$$

where $\{y_r\}$ is a wide sense stationary time series with zero mean, unit variance and independent samples, then $E(x_r x_{r+j}) = \phi_j$; thus, T_n is the autocovariance matrix of any $n + 1$ successive samples of $\{x_r\}$.

Rehnqvist's procedure requires multiplying T_n by matrices whose forms depend strongly on the residue class of n modulo m. This can be avoided by using Theorems 1 and 2. If ϕ_j is given by (20), the characteristic polynomial of (11) is

$$z^{m-1} \sum_{j=-m+1}^{m-1} \phi_j z^j = m^{-1}(1-z)^{-2}(1-z^m)^2;$$

thus

$$\psi_{r,n-1} = \sum_{j=1}^{m-1} (B_{j,n-1} + rC_{j,n-1}) \exp(2\pi irj/m),$$

where $\{B_{j,n-1}\}$ and $\{C_{j,n-1}\}$ are to be determined from (12). This problem is a special case of one solved in [6] in connection with linear minimum variance prediction of x_{r+k} based on observed values of $x_r, x_{r-1}, \cdots, x_{r-n+1}$. Since $\sum_{j=0}^{n-1} \psi_{j,n-1} x_{r-j}$ is the best such estimate of x_{r+1}, the results of [6] apply here. The pertinent results follow.

Case 1. If $n \equiv 0 \pmod{m}$, then

$$\psi_{j,n-1} = (n-j)/(n+1) \quad \text{if } j \equiv 0 \pmod{m},$$
$$\psi_{j,n-1} = -(n-j)/(n+1) \quad \text{if } j \equiv -1 \pmod{m},$$
$$\psi_{j,n-1} = 0 \quad\quad\quad \text{otherwise};$$
$$\Delta_{n-1} = (n+m)/m(n+1).$$

Case 2. If $n \equiv 1 \pmod{m}$, then

$$\psi_{j,n-1} = (n+m-j-2)/(n+m-1) \quad \text{if } j \equiv 0 \pmod{m},$$
$$\psi_{j,n-1} = -(n+m-j-2)/(n+m-1) \quad \text{if } j \equiv -1 \pmod{m},$$
$$\psi_{j,n-1} = 0 \quad\quad\quad\quad \text{otherwise};$$
$$\Delta_{n-1} = (n+2m-2)/m(n+m-1).$$

Case 3. If $n \equiv k \pmod{m}$, where $2 \leqslant k \leqslant m-1$, then

$$\psi_{j,n-1} = \frac{(n+2m-2k)(n+m-k-j)}{(n+m-k)(n+2m-2k+1)} \quad \text{if } j \equiv 0 \pmod{m},$$

$$\psi_{j,n-1} = \frac{-(m-k+j+1)}{(n+m-k)(n+2m-2k+1)} \quad \text{if } j \equiv k-1 \pmod{m},$$

$$\psi_{j,n-1} = -\frac{(n+m-k-j-1)}{(n+m-k)} \quad \text{if } j \equiv -1 \pmod{m},$$

$$\psi_{j,n-1} = 0 \quad \text{otherwise};$$

$$\Delta_{n-1} = \frac{(n+2m-2k)(n+2m-k)}{m(n+m-k)(n+2m-2k+1)}.$$

Since T_n is symmetric, $\eta_{r,n-1} = \psi_{r,n-1}$ and T_n^{-1} can now be computed from (5)–(8).

4. The Modified Algorithm for $\{\psi_{r,n-1}\}$ **and** $\{\eta_{r,n-1}\}$. Even if the difference equations of Theorem 2 cannot conveniently be solved explicitly, they still provide a useful simplification in computing T_n^{-1}, as we now show.

The algorithm of [5] includes a recursive procedure for computing $\psi_{0,n-1}, \cdots,$ $\psi_{n-1,n-1}$ and $\eta_{0,n-1}, \cdots, \eta_{n-1,n-1}$ with $O(n^2)$ operations, provided $T_0, \cdots,$ T_{n-1} are all nonsingular. For band matrices, this can be done with $O(n)$ operations.

THEOREM 3. *Let* $p + q \leqslant k < n - 1$. *If* $T_k, T_{k+1}, \cdots, T_{n-1}$ *are all nonsingular, then* $\psi_{0,n-1}, \cdots, \psi_{n-1,n-1}$ *and* $\eta_{0,n-1}, \cdots, \eta_{n-1,n-1}$ *can be computed as follows.*

(a) *Obtain* $\psi_{0k}, \cdots, \psi_{kk}$ *and* $\eta_{0k}, \cdots, \eta_{kk}$ *by solving* (3) *and* (4) *with* $n - 1 = k$, *and compute*

$$\Delta_k = \phi_0 - \sum_{r=0}^{q-1} \phi_{-r-1} \psi_{r,k}$$

or, equivalently,

$$\Delta_k = \phi_0 - \sum_{r=0}^{p-1} \phi_{r+1} \eta_{r,k}.$$

(b) *For* $k + 1 \leqslant m \leqslant n - 1$, *compute*

$$\psi_{mm} = -\Delta_{m-1}^{-1} \sum_{s=m-p}^{m-1} \psi_{s,m-1} \phi_{m-s};$$

$$\eta_{mm} = -\Delta_{m-1}^{-1} \sum_{s=m-q}^{m-1} \eta_{s,m-1} \phi_{-m+s};$$

(21) $$\psi_{rm} = \psi_{r,m-1} - \psi_{mm} \eta_{m-r-1,m-1}$$

for $0 \leqslant r \leqslant q - 1$ *and* $m - p + 1 \leqslant r \leqslant m - 1$;

(22) $$\eta_{rm} = \eta_{r,m-1} - \eta_{mm} \psi_{m-r-1,m-1}$$

for $0 \leqslant r \leqslant p - 1$ *and* $m - q + 1 \leqslant r \leqslant m - 1$; *and* $\Delta_m = (1 - \psi_{mm}\eta_{mm})\Delta_{m-1}$.

(c) *Then compute*

(23)
$$\psi_{r,n-1} = -\frac{1}{\phi_{-q}} \sum_{j=-p}^{q-1} \phi_{-j} \psi_{r-q+j,n-1}$$

for $q \leqslant r \leqslant m - p$, with $\psi_{j,n-1} = -\delta_{-1,j}$ for $-p \leqslant j \leqslant -1$, and

(24)
$$\eta_{r,n-1} = -\frac{1}{\phi_p} \sum_{j=-q}^{p-1} \phi_j \eta_{r-p+j,n-1}$$

for $p \leqslant r \leqslant m - q$, with $\eta_{j,n-1} = -\delta_{-1,j}$ for $-q \leqslant j \leqslant -1$.

This theorem follows from Theorem 2 and recursion formulas given in [5] for $\{\psi_{rm}\}$ and $\{\eta_{rm}\}$. A special case of Theorem 3 for hermitian T_n was stated in [7] in connection with minimum variance prediction of finite moving-average processes.

The essential difference between Theorem 3 and the general algorithm of [5] is that (23) and (24) are not available in the latter, and it is necessary to use (21) and (22) for m values $(0 \leqslant r \leqslant m - 1)$ each, rather than $p + q$.

5. **Comments.** In using Theorem 1, it is worthwhile to note that T_n^{-1} is symmetric about its secondary diagonal; i.e., $b_{n-s,n-r,n} = b_{rsn}$. If $\phi_{-j} = \overline{\phi_j}$, then T_n^{-1} is also hermitian; moreover, the computations in Theorems 1, 2 and 3 are, in this case, further shortened by the fact that $\psi_{rm} = \overline{\eta}_{rm}$.

Throughout this paper, we have excluded the case where $p = 0$ or $q = 0$, so that T_n is triangular. Inversion of a nonsingular triangular Toeplitz matrix—band or not—is very simple: if

(25)
$$\phi_j = 0, \quad j < 0,$$

and (without loss of generality) $\phi_0 = 1$, then T_n^{-1} is the Toeplitz matrix given by

(26)
$$b_{rsn} = -\psi_{r-s-1},$$

with $\psi_j = 0$ if $j < -1$, $\psi_{-1} = -1$, and

(27)
$$\psi_j = \phi_{j+1} - \sum_{s=0}^{j-1} \phi_{j-s} \psi_s, \quad 0 \leqslant j \leqslant n - 1.$$

To see this, note that (4) and (25) imply that $\eta_{s,n-1} = 0$ and that (3) is a triangular system with solution (27). Now, (26) follows from (5)–(8).

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