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Explicit inverses of Toeplitz and associated matrices

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Abstract

We discuss Toeplitz and associated matrices which have simple explicit expressions for their inverses. We first review existing results and generalize these where possible, including matrices with hyperbolic and trigonometric elements. In §2 we discuss and generalize the Fiedler matrix. In §3 we give an analytic procedure for inverting any band Toeplitz matrix, in §4 we invert a tridiagonal Toeplitz matrix with modified corner elements.

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1 Introduction and review

Toeplitz matrices were originally studied by Toeplitz [18, 29] who called the related quadratic form an *L-form*. A Toeplitz matrix is of the form $A_{ij} = c_{i-j}$ with c_{-m} the complex conjugate of c_m, and they occur in many fields [13, 22]. Here we report the results of our search for real Toeplitz matrices with simple explicit inverses.

The matrices in this paper occur in many applications, and they are useful as test matrices for numerical routines. Band matrices in particular occur frequently in linear equations; however, solution via a Gaussian elimination method is usually preferable to using a dense inverse, except when only a few elements of the solution are required.

For example when solving the n linear equations $Ax = b$, where A is the band matrix in §3.3, but only require x_1, we have the exact

$$x_1 = \frac{1}{(n+2)(n+3)} \sum_{j=1}^{n} j(n+1-j)(n+2-j)b_j$$

which is $5n+2$ flops, compared to about $16n$ flops for Gaussian elimination.

There are times when an explicit inverse is required; for example the determinant can usually be found once the inverse is known, as is done in some of the proofs in this paper. See also [2, 7, 20]. Portions of explicit inverses can also be used as pre-conditioners for the conjugate gradient method [8].

In section §1 we review existing results and generalize these, notably finding the hyperbolic and trigonometric matrices, and in §2 we generalize Fiedler's matrix [28]. While Fiedler's matrix is not in general a Toeplitz matrix, it is closely related to a Toeplitz matrix; for example its inverse has the same sparsity pattern as many of the matrices in §1.

In §3 we give a simple method for finding the inverse of a band Toeplitz matrix, which differs from Rozsa's [24] approach. We use these results to derive the inverse of a tridiagonal Toeplitz matrix, taking care to consider all possible values of the diagonals. These methods can be used to find the eigenvalues of these matrices (or an expression proportional to the characteristic polynomial); however the algebra is prohibitive except for very small bandwidth. Other methods, for example solving the recurrence relation in x that is implicit in the eigenvalue equation $Ax - \lambda x = 0$ [19] or via determinants [9, 26], provide a more direct way to the characteristic polynomial. We find that the solutions of the recurrence (4) provide 'basis functions' for the elements of A^{-1}.

In §4 we illustrate the flexibility of this approach by deriving the inverse of a tridiagonal matrix with constant diagonals, but with modified corner elements.

In this paper we denote the order of the matrix A by n. We begin by quoting examples from the literature.

1.1 Matrix 1: $c + d|i - j|$

In [28] the inverse of the matrix $A_{ij} = |i - j|$, $i, j = 1, \ldots, n$ was given; we generalize this ($n > 2$) to the matrix:

$$A_{ij} = \begin{cases} c + d_1|i-j|, & i \le j, \quad i,j = 1,\ldots,n \\ c + d_2|i-j|, & i \ge j, \quad i,j = 1,\ldots,n \end{cases}$$

which has the inverse

$$A^{-1} = \frac{1}{d_1 + d_2} \begin{bmatrix} -\xi_{n-1}/\xi_n & 1 & 0 & \cdots & 0 & d_1^2/\xi_n \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & 1 & -2 & 1 \\ d_2^2/\xi_n & 0 & \cdots & 0 & 1 & -\xi_{n-1}/\xi_n \end{bmatrix}$$

where $\xi_n = c(d_1 + d_2) + d_1 d_2 (n - 1)$ (see also [12, pp31,51] and [27]).

We shall see this sparsity pattern several times in this paper, namely tridiagonal with constant diagonals except for the corner elements, and we shall see that this matrix is a particular case of the generalized Fiedler matrix discussed in §2. The determinant is $|A| = -(-1)^n(d_1+d_2)^{n-2}\xi_n$.

A band matrix form of this, namely $A_{ij} = k-|i-j|$ for $|i-j| < k$, zero otherwise, was inverted in [21].

1.2 Matrix 2: $(-1)^{i-j}(c+d|i-j|)$

The corresponding result, in which the three diagonals of the inverse have the same sign is of interest ($n > 2$):

$$A_{ij} = \begin{cases} (-1)^{i-j}(c+d_1|i-j|), & i \le j, \quad i,j = 1,\dots,n \\ (-1)^{i-j}(c+d_2|i-j|), & i \ge j, \quad i,j = 1,\dots,n \end{cases} \tag{1}$$

has the inverse

$$A^{-1} = -\frac{1}{d_1+d_2}\begin{bmatrix} \xi_{n-1}/\xi_n & 1 & 0 & \cdots & 0 & (-)^n d_1^2/\xi_n \\ 1 & 2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & 2 & 1 & 0 & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & 1 & 2 & 1 \\ (-)^n d_2^2/\xi_n & \cdots & 0 & 0 & 1 & \xi_{n-1}/\xi_n \end{bmatrix}$$

where ξ_n and the determinant are the same as for Matrix 1.

1.3 KMS matrix: $\rho^{|i-j|}$

The Kac-Murdock-Szegö matrix is the symmetric Toeplitz matrix [13, 18, 33] ($\rho \ne 1$, $n > 1$):

$$A_{ij} = \rho^{|i-j|}, \quad i,j = 1,\dots,n$$

It has the simple tridiagonal inverse

$$A^{-1} = \frac{1}{1-\rho^2}\begin{bmatrix} 1 & -\rho & 0 & \cdots & 0 \\ -\rho & 1+\rho^2 & -\rho & \cdots & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & \cdots & -\rho & 1+\rho^2 & -\rho \\ 0 & \cdots & 0 & -\rho & 1 \end{bmatrix}.$$

The determinant is $|A| = (1-\rho^2)^{n-1}$. For a Matlab program which generates the LU decomposition of this matrix, see `kms.m` in [15], and for its eigenvalues see [13, p69]. This is the only form of a symmetric Toeplitz matrix whose inverse is a tridiagonal matrix; this can be shown by using the result that the inverse of a symmetric irreducible nonsingular tridiagonal matrix T is of the general form [2, 4, 5, 23, 24]

$$T^{-1}_{ij} = \begin{cases} u_i v_j\,, & i \le j \\ u_j v_i\,, & i > j \end{cases} \tag{2}$$

The matrix P of [34] is a KMS matrix, except it differs by the factor ρ^{n-1}, with $\rho = 1/q$. Given the matrix T the vectors u, v are easy to derive, see §3.1 or [8]; this and similar results are constantly being rediscovered [7, 17, 35, e.g.].

The KMS matrix and some of its generalizations given below are semiseparable matrices [10].

1.4 Nonsymmetric KMS matrix

The nonsymmetric version of the KMS matrix is:

$$A_{ij} = \begin{cases} \rho^{j-i}, & i < j\,, \quad i,j = 1,\dots,n \\ \sigma^{i-j}, & i > j\,, \quad i,j = 1,\dots,n \\ 1\,, & i = j\,. \end{cases}$$

Its inverse is

$$A^{-1} = \frac{1}{1-\sigma\rho}\begin{bmatrix} 1 & -\rho & 0 & \cdots & 0 \\ -\sigma & 1+\sigma\rho & -\rho & \cdots & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & \cdots & -\sigma & 1+\sigma\rho & -\rho \\ 0 & \cdots & 0 & -\sigma & 1 \end{bmatrix}.$$

The determinant is $|A| = (1-\sigma\rho)^{n-1}$.

1.5 Generalized KMS matrix: $\alpha + \beta\rho^{|i-j|}$

A generalized symmetric KMS matrix is:

$$A_{ij} = \begin{cases} \alpha + \beta\rho^{|i-j|}, & i,j = 1,\ldots,n \\ \alpha + \beta\,, & i = j \end{cases}$$

Its inverse is

$$A^{-1} = \frac{1}{f_n(1-\rho^2)}\begin{bmatrix} d_0 & a_0 & b & \cdots & b & b & c \\ a_0 & d & a & e & \cdots & e & b \\ b & a & d & a & e & \cdots & b \\ & & & \ddots & \ddots & \ddots & \\ b & e & \cdots & e & a & d & a_0 \\ c & b & b & \cdots & b & a_0 & d_0 \end{bmatrix}. \qquad (3)$$

where

$$\begin{aligned} d &= -1-\rho-\rho^2-\rho^3+\alpha\{-n_1+n_5\rho-n_3\rho^2(1-\rho)\}/\beta \\ a &= \rho(1+\rho)+\alpha(1+n_3\rho-n_5\rho^2-\rho^3)/\beta \\ a_0 &= \rho(1+\rho)+\alpha(1+n_2\rho-n_3\rho^2)/\beta \\ d_0 &= -1-\rho+\alpha(n_3\rho-n_1)/\beta \end{aligned}$$

$b=(1-\rho)^2\alpha/\beta$, $c=(1-\rho)\alpha/\beta$, $e=(1-\rho)^3\alpha/\beta$, $n_m=n-m$, $f_n=-n\alpha-\beta(1+\rho)+n_2\alpha\rho$. For example ($n=8$, $\alpha=1$, $\beta=2$, $\rho=2$):

$$A^{-1}=\begin{bmatrix} 3 & 5 & 9 & 17 & 33 & 65 & 129 & 257 \\ 5 & 3 & 5 & 9 & 17 & 33 & 65 & 129 \\ 9 & 5 & 3 & 5 & 9 & 17 & 33 & 65 \\ 17 & 9 & 5 & 3 & 5 & 9 & 17 & 33 \\ 33 & 17 & 9 & 5 & 3 & 5 & 9 & 17 \\ 65 & 33 & 17 & 9 & 5 & 3 & 5 & 9 \\ 129 & 65 & 33 & 17 & 9 & 5 & 3 & 5 \\ 257 & 129 & 65 & 33 & 17 & 9 & 5 & 3 \end{bmatrix}^{-1}$$

$$=-\frac{1}{12}\begin{bmatrix} 3 & -5 & -1 & -1 & -1 & -1 & -1 & 1 \\ -5 & 11 & -3 & 1 & 1 & 1 & 1 & -1 \\ -1 & -3 & 11 & -3 & 1 & 1 & 1 & -1 \\ -1 & 1 & -3 & 11 & -3 & 1 & 1 & -1 \\ -1 & 1 & 1 & -3 & 11 & -3 & 1 & -1 \\ -1 & 1 & 1 & 1 & -3 & 11 & -3 & -1 \\ -1 & 1 & 1 & 1 & 1 & -3 & 11 & -5 \\ 1 & -1 & -1 & -1 & -1 & -1 & -5 & 3 \end{bmatrix}$$

We have quoted this matrix partly because its inverse, which although dense depends on only seven parameters, has a form which occurs in other cases. We quote four of these:

1. the centrosymmetric [3] Toeplitz matrix ($n>2$, $d\neq 0$)

$$A_{ij}=c+d\,|i-j|+e\,(i-j)^2,\quad i,j=1,\ldots,n\,;$$

2. the matrix

$$A_{ij}=c+d(-1)^{i-j}|i-j|,\quad i,j=1,\ldots,n$$

which is apparently similar to (1) but whose inverse is dense;

3. the matrix

$$A_{ij} = c + (-1)^{i-j}\{d\,|i-j| + e\,(i-j)^2\}, \quad i,j = 1,\ldots,n\,;$$

4. and finally the matrix

$$A_{ij} = d + \alpha\sin(\rho|i-j|) + \beta\cos(\rho|i-j|), \quad i,j = 1,\ldots,n\,.$$

Because the inverse of these matrices has the form (3) it is not difficult to find explicit expressions for their inverses. We can also obtain expressions for the nonsymmetric case but they are somewhat more complex.

For another generalization of the KMS matrix, see [30].

1.6 Hyperbolic matrix: $\alpha\rho^{-|i-j|} + \beta\rho^{|i-j|}$

The symmetric Toeplitz matrix

$$A_{ij} = \begin{cases} \alpha\rho^{-|i-j|} + \beta\rho^{|i-j|} & i,j = 1,\ldots,n \\ \alpha+\beta & i = j \end{cases}$$

has the inverse

$$A^{-1} = \frac{1}{(\alpha-\beta)(\rho^2-1)} \begin{bmatrix} d_0 & -\rho & 0 & \cdots & 0 & c \\ -\rho & 1+\rho^2 & -\rho & 0 & \cdots & 0 \\ 0 & -\rho & 1+\rho^2 & -\rho & 0 & \cdots \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & -\rho & 1+\rho^2 & -\rho \\ c & 0 & \cdots & 0 & -\rho & d_0 \end{bmatrix}$$

where $d_0 = \rho^2 f_{2n-4}/f_{2n-2}$, $c = \alpha\beta\rho^{n-1}(1-\rho^2)/f_{2n-2}$ and $f_k = \alpha^2 - \beta^2\rho^k$.

The determinant of A is $|A| = (\alpha-\beta)^{n-2}(\rho^2-1)^{n-1} f_{2n-2}/\rho^{2n-2}$.

We now write A in terms of hyperbolic functions, partly for reasons of comparison with the next section, but also because of the beauty of the matrix; we also generalize to a nonsymmetric matrix:

$$A_{ij} = \begin{cases} \alpha\sinh(\rho|i-j|) + \beta\cosh(\rho|i-j|) & i \le j,\ i,j = 1,\ldots,n, \\ \gamma\sinh(\rho|i-j|) + \beta\cosh(\rho|i-j|) & i \ge j,\ i,j = 1,\ldots,n, \end{cases}$$

which has the inverse

$$A^{-1} = \frac{1}{\alpha+\gamma}\begin{bmatrix} d_0 & a & 0 & \cdots & 0 & f \\ a & d & a & 0 & \cdots & 0 \\ 0 & a & d & a & \cdots & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & a & d & a \\ e & 0 & \cdots & 0 & a & d_0 \end{bmatrix}$$

where

$$\begin{aligned} a &= \operatorname{csch}\rho \\ d &= -2\coth\rho \\ e &= -(\beta g_{n-2}\operatorname{csch}\rho + g_{n-1}(\gamma-\beta\coth\rho)/D \\ f &= -(\beta h_{n-2}\operatorname{csch}\rho + h_{n-1}(\alpha-\beta\coth\rho)/D \\ d_0 &= (g_{n-2}h_{n-1}\operatorname{csch}\rho + \beta(\gamma-\beta\coth\rho))/D \\ D &= \beta^2 - g_{n-1}h_{n-1} \\ h_k &= \alpha\sinh(\rho k) + \beta\cosh(\rho k) \\ g_k &= \gamma\sinh(\rho k) + \beta\cosh(\rho k) \end{aligned}$$

As we shall see this has a perfect analogue in the trigonometric functions.

1.7 Trigonometric matrix: $\alpha \sin(\rho|i-j|) + \beta \cos(\rho|i-j|)$

The previous matrix leads to our next matrix: the nonsymmetric trigonometric Toeplitz matrix

$$A_{ij} = \begin{cases} \alpha \sin(\rho|i-j|) + \beta \cos(\rho|i-j|) & i \leq j, \ i,j = 1,\ldots,n \\ \gamma \sin(\rho|i-j|) + \beta \cos(\rho|i-j|) & i \geq j, \ i,j = 1,\ldots,n \end{cases}$$

which has the inverse

$$A^{-1} = \frac{1}{\alpha+\gamma} \begin{bmatrix} d_0 & a & 0 & \cdots & 0 & f \\ a & d & a & 0 & \cdots & 0 \\ 0 & a & d & a & \cdots & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & a & d & a \\ e & 0 & \cdots & 0 & a & d_0 \end{bmatrix}$$

where

$$\begin{aligned} a &= \csc\rho \\ d &= -2\cot\rho \\ e &= -(\beta g_{n-2}\csc\rho + g_{n-1}(\gamma - \beta\cot\rho)/D \\ f &= -(\beta h_{n-2}\csc\rho + h_{n-1}(\alpha - \beta\cot\rho)/D \\ d_0 &= (g_{n-2}h_{n-1}\csc\rho + \beta(\gamma - \beta\cot\rho))/D \\ D &= \beta^2 - g_{n-1}h_{n-1} \\ h_k &= \alpha\sin(\rho k) + \beta\cos(\rho k) \\ g_k &= \gamma\sin(\rho k) + \beta\cos(\rho k) \end{aligned}$$

The curious thing about this matrix is that the asymmetry is confined to the corner elements e and f. We will quote a (symmetric) example: let $n = 8$, $\alpha = \beta = \gamma = 1$, $\rho = \pi/4$ then

$$A^{-1} = \begin{bmatrix} 1 & \sqrt{2} & 1 & 0 & -1 & -\sqrt{2} & -1 & 0 \\ \sqrt{2} & 1 & \sqrt{2} & 1 & 0 & -1 & -\sqrt{2} & -1 \\ 1 & \sqrt{2} & 1 & \sqrt{2} & 1 & 0 & -1 & -\sqrt{2} \\ 0 & 1 & \sqrt{2} & 1 & \sqrt{2} & 1 & 0 & -1 \\ -1 & 0 & 1 & \sqrt{2} & 1 & \sqrt{2} & 1 & 0 \\ -\sqrt{2} & -1 & 0 & 1 & \sqrt{2} & 1 & \sqrt{2} & 1 \\ -1 & -\sqrt{2} & -1 & 0 & 1 & \sqrt{2} & 1 & \sqrt{2} \\ 0 & -1 & -\sqrt{2} & -1 & 0 & 1 & \sqrt{2} & 1 \end{bmatrix}^{-1}$$

$$= \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & -\sqrt{2} & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -\sqrt{2} & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -\sqrt{2} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -\sqrt{2} & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -\sqrt{2} & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -\sqrt{2} & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

2 Fiedler's matrix: $c_j - c_i$

In a surprising result, Fiedler [28], stated that the inverse of

$$C_{ij} = \begin{cases} c_j - c_i, & i < j, \quad i, j = 1, \ldots, n \\ c_i - c_j, & i > j, \quad i, j = 1, \ldots, n \\ 0, & i = j, \end{cases}$$

$(n > 2)$ is also given by a tridiagonal matrix except for c_{1n}^{-1} and $c_{n1}^{-1} \neq 0$: Put $d_1 = 1/(c_1 - c_2) - 1/(c_1 - c_n)$, $d_i = 1/(c_{i-1} - c_i) + 1/(c_i - c_{i+1})$,

$i = 2, \ldots, n-1$, $d_n = 1/(c_{n-1} - c_n) - 1/(c_1 - c_n)$, then

$$C_{ij}^{-1} = \frac{1}{2}\begin{bmatrix} d_1 & \frac{1}{c_2-c_1} & 0 & \cdots & 0 & \frac{1}{c_n-c_1} \\ \frac{1}{c_2-c_1} & d_2 & \frac{1}{c_3-c_2} & 0 & \cdots & 0 \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & \frac{1}{c_{n-1}-c_{n-2}} & d_{n-1} & \frac{1}{c_n-c_{n-1}} \\ \frac{1}{c_n-c_1} & 0 & \cdots & 0 & \frac{1}{c_n-c_{n-1}} & d_n \end{bmatrix}$$

We have printed this in full as there was a slight error in the original publication. Fiedler also gave an expression for the determinant of this matrix: $|C| = -(-1)^n 2^{n-2} \prod_{j=1}^{n-1}(c_{j+1} - c_j)(c_n - c_1)$, $(n > 1)$.

2.1 Generalized nonsymmetric Fiedler's matrix: $d + pc_i + qc_j$

We have generalized Fiedler's matrix to:

$$C_{ij} = \begin{cases} d + pc_i + qc_j\,, & i < j, \quad i, j = 1, \ldots, n \\ d + rc_i + sc_j\,, & i > j, \quad i, j = 1, \ldots, n \\ d + (p+q)c_i\,, & i = j, \end{cases}$$

where we require $r + s = p + q$ to make the upper and lower triangles consistent. The inverse is very similar to Fiedler's matrix. Put

$$\begin{aligned} e &= sr/\xi_{1n} \\ f &= pq/\xi_{1n} \\ d_1 &= \frac{\xi_{2n}}{(c_1 - c_2)\,\xi_{1n}} \\ d_n &= \frac{\xi_{1n-1}}{(c_{n-1} - c_n)\,\xi_{1n}} \\ \xi_{ij} &= d\,(p - r) + psc_i - qrc_j \end{aligned}$$

otherwise d_i is as above, then provided C^{-1} exists, for $n > 2$ it is given by

$$C^{-1}_{ij} = \frac{1}{r-p}\begin{bmatrix} d_1 & \frac{1}{c_2-c_1} & \cdots & 0 & f \\ \frac{1}{c_2-c_1} & d_2 & \frac{1}{c_3-c_2} & \cdots & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & \cdots & \frac{1}{c_{n-1}-c_{n-2}} & d_{n-1} & \frac{1}{c_n-c_{n-1}} \\ e & 0 & \cdots & \frac{1}{c_n-c_{n-1}} & d_n \end{bmatrix}$$

Example: $n = 8$, $d = 2$, $p = 1$, $q = 1$, $r = 4$, and $c = \{\ 1\ \ 2\ \ 0\ \ 1\ \ 2\ \ 0\ \ 1\ \ 2\ \}$:

$$A^{-1} = \begin{bmatrix} 4 & 5 & 3 & 4 & 5 & 3 & 4 & 5 \\ 8 & 6 & 4 & 5 & 6 & 4 & 5 & 6 \\ 0 & -2 & 2 & 3 & 4 & 2 & 3 & 4 \\ 4 & 2 & 6 & 4 & 5 & 3 & 4 & 5 \\ 8 & 6 & 10 & 8 & 6 & 4 & 5 & 6 \\ 0 & -2 & 2 & 0 & -2 & 2 & 3 & 4 \\ 4 & 2 & 6 & 4 & 2 & 6 & 4 & 5 \\ 8 & 6 & 10 & 8 & 6 & 10 & 8 & 6 \end{bmatrix}^{-1}$$

$$= \frac{1}{6}\begin{bmatrix} -2\frac{1}{4} & 2 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{8} \\ 2 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & -1 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & -4 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & -4 & 2 \\ 1 & 0 & 0 & 0 & 0 & 0 & 2 & -1\frac{1}{2} \end{bmatrix}$$

The only further generalization of this matrix which still has a sparse inverse that we have found at this stage is to add the rank one term: $+\rho c_i c_j$ to C. The matrices of §1.1 and §1.2 are instances of a Fiedler matrix.

3 Inverse of band Toeplitz matrix

Rozsa [24] gave formulae for the inverses of band matrices; we will derive equivalent results in a different and more direct way; note that our definition of p and q is different to Rozsa. In his treatment, he has to evaluate $4(p+q)$ determinants of order $p+q$, whereas here we need to solve two systems of order $p+q$. The terms in Rozsa's expression for the inverse are more concise, being sums of rank p or q (which agrees with Barrett [6]), whereas here we derive sums of $p+q$ terms.

Consider the band Toeplitz matrix

$$A = \begin{bmatrix} c_0 & c_1 & \cdots & c_q & 0 & 0 \\ c_{-1} & c_0 & c_1 & \cdots & c_q & 0 \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & c_{-p} & \cdots & c_0 & c_1 \\ 0 & 0 & \cdots & c_{-p} & \cdots & c_0 \end{bmatrix}$$

where $p \geq 0$, $q \geq 0$, $p+q \geq 1$. That is

$$A_{ij} = \begin{cases} c_{j-i}\,, & -p \leq j-i \leq q \\ 0\,, & \text{otherwise.} \end{cases}$$

We invert this matrix using solutions to the difference equation (4).

Theorem 1 *1. Let $r_k(i)$, $k = 1, \ldots, p+q$ be a set of $p+q$ linearly independent solutions to the difference equation*

$$c_{-p}r(i-p) + c_{1-p}r(i-p+1) + \cdots + c_q r(i+q) = 0\,, \qquad (4)$$

for $i = \ldots, 0, 1, 2, \ldots$

2. *Construct two solutions to (4):*

$$P_{ij} = \sum_{k=1}^{p+q} a_k(j) r_k(i)\,;$$

$$Q_{ij} = \sum_{k=1}^{p+q} \left[a_k(j) - z_k(j)\right] r_k(i)\,. \tag{5}$$

3. *To find a_k and z_k solve:*

$$\begin{aligned} P_{ij} &= 0\,, \quad i = 1-p, \ldots, 0, \quad \text{if } p > 0\,; && (6)\\ Q_{ij} &= 0\,, \quad i = n, \ldots, n+q, \quad \text{if } q > 0\,; && (7)\\ P_{ij} &= Q_{ij}\,, \quad i = j-p+1, \ldots, j+q-1, \\ &\qquad \text{if } p+q > 1\,; && (8) \end{aligned}$$

$$c_{-p}A^{-1}_{j-p,j} + c_{1-p}A^{-1}_{j-p+1,j} + \cdots + c_q A^{-1}_{j+q,j} = 1\,. \tag{9}$$

Since P satisfies (4) the last condition becomes

$$-P_{j+q,j} + Q_{j+q,j} = 1/c_q\,, \qquad \text{if } p+q > 1\,. \tag{10}$$

We assert that the inverse of A is

$$A^{-1}_{ij} = \begin{cases} P_{ij}\,, & 1 \le i \le j+q-1 \\ Q_{ij}\,, & j-p+1 \le i \le n \end{cases} \tag{11}$$

Proof: Because P, Q as functions of i satisfy the difference equation (4) it is clear that $B_{ij} = \sum A_{ik}P_{kj}$ (or $A_{ik}Q_{kj}$) will be zero in general except perhaps for i near 1 or n. Equations (6) and (7) ensure that $B_{ij} = 0$ for $i < p+1$ or $i > n-q$. Next, (10) ensures that $B_{ii} = 1$, and finally (8) ensures that P and Q are consistent over their common domain. Hence $B = I$ and we have constructed the inverse of A. ♠

Because of the way we chose a_k and z_k, the system (6–10) of $2(p+q)$ equations for $a_k(j)$ and $z_k(j)$ separates into two systems of size $p+q$.

To solve these, first we solve equations (8) and (10)

$$\sum_{k=1}^{p+q} r_k(j-p+l)z_k(j) = \begin{cases} 0\,, & l=1,\ldots,p+q-1 \\ -1/c_q\,, & l=p+q \end{cases} \tag{12}$$

These will always be solvable as the r_k are linearly independent. Then we solve the $p+q$ equations

$$\sum_{k=1}^{p+q} r_k(l)a_k(j) = \begin{cases} 0\,, & l=1-p,\ldots,0 \\ \sum_{k=1}^{p+q} r_k(l)z_k(j)\,, & l=n+1,\ldots,n+q \end{cases} \tag{13}$$

These equations should be solved symbolically, giving explicit expressions for $a_k(j)$ and $z_k(j)$ and hence P and Q, in terms of i and j.

We also note that if A is singular then the determinant

$$|r_k(l)| = 0 \tag{14}$$

where $l = 1-p,\ldots,0,\ n+1,\ldots,n+q$. The reverse of this is not necessarily true, thus (14) can have parasitic solutions, which correspond to the occurrence of equal roots of (4). Thus we can use (14) to obtain the eigenvalues of A, if we replace c_0 by $c_0-\lambda$. We do not need to solve (4) directly; rather we use symmetric functions of the roots of (4) to simplify (14), for example if (4) has the solutions $r(i)=r_k^i$ then we have $\prod r_k = (-)^{p+q}c_{-p}/c_q$. We will not explore this technique further, as other methods [19, 25] are more direct.

3.1 Example: General tridiagonal matrix

Consider the tridiagonal matrix

$$A = \begin{bmatrix} c_0 & c_1 & 0 & \cdots & 0 & 0 \\ c_{-1} & c_0 & c_1 & 0 & \cdots & 0 \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & c_{-1} & c_0 & c_1 \\ 0 & 0 & \cdots & 0 & c_{-1} & c_0 \end{bmatrix}.$$

Many authors have inverted particular cases of this matrix [20], but for the convenience of the reader we quote the general solution. To find the inverse of A we first solve (4) in the usual way, putting $r(i) = r^i$, giving $c_{-1} + rc_0 + r^2 c_1 = 0$. We need to consider three cases: two unequal real roots, two equal roots or two complex roots. We have $p = q = 1$. First we solve (12) giving

$$\begin{aligned} z_1(j) &= -r_2(j)/c_1 D(j)\,, \\ z_2(j) &= r_1(j)/c_1 D(j)\,, \end{aligned}$$

where

$$D(j) = r_1(j+1) r_2(j) - r_1(j) r_2(j+1)\,.$$

We then solve (13) for the three cases, the inverse being given by (11).

Unequal real roots The roots are $r_1, r_2 = (-c_0 \pm \sqrt{c_0^2 - 4c_{-1}c_1})/2c_1$, and $r_k(i) = r_k^i$, $r_1 \neq r_2$. Then

$$P_{ij} = -\frac{(r_1^i - r_2^i)(r_1^{n+1-j} - r_2^{n+1-j})}{c_1 (r_1 - r_2)(r_1^{n+1} - r_2^{n+1})}\,,$$

$$Q_{ij} = \frac{(r_1^{-j} - r_2^{-j})(r_1^{n+1} r_2^i - r_2^{n+1} r_1^i)}{c_1(r_1 - r_2)(r_1^{n+1} - r_2^{n+1})} \,. \tag{15}$$

We also record the latter in a form emphasising the symmetry:

$$Q_{ij} = -\frac{(r_1^j - r_2^j)(r_1^{n+1-i} - r_2^{n+1-i})}{c_1(r_1 - r_2)(r_1^{n+1} - r_2^{n+1})} \left(\frac{c_{-1}}{c_1}\right)^{i-j} \,.$$

Haley [14] gave these in terms of hyperbolic functions, and we quote them here for completeness. We assume without loss of generality that $c_0 > 0$. Put $\cosh\theta = c_0/2\sqrt{c_{-1}c_1}$, $r = -\sqrt{c_{-1}/c_1}$ if $c_1 > 0$ and $r = \sqrt{c_{-1}/c_1}$ if $c_1 < 0$. Then

$$P_{ij} = \frac{r^{i-j}\sinh i\theta \ \sinh(n+1-j)\theta}{\sqrt{c_{-1}c_1}\sinh\theta \ \sinh(n+1)\theta} \,,$$

$$Q_{ij} = \frac{r^{i-j}\sinh j\theta \ \sinh(n+1-i)\theta}{\sqrt{c_{-1}c_1}\sinh\theta \ \sinh(n+1)\theta} \,. \tag{16}$$

These formulae still apply if $c_{-1}c_1 < 0$ but because of the imaginary terms, (15) is to be preferred.

Equal roots Here $r_1(i) = r^i$, $r_2(i) = ir^i$, $r = -c_0/2c_1$. Then

$$P_{ij} = -\frac{2r^{i-j} i(j-n-1)}{c_0(n+1)} \,,$$

$$Q_{ij} = -\frac{2r^{i-j} j(i-n-1)}{c_0(n+1)} \,.$$

Complex roots Here $r_1(i) = r^i\cos i\theta$, $r_2(i) = r^i\sin i\theta$, where $r = \sqrt{c_{-1}/c_1}$, $\cos\theta = -c_0/2rc_1$. Then

$$P_{ij} = -\frac{r^{i-j}\sin i\theta \ \sin(n+1-j)\theta}{\sqrt{c_{-1}c_1}\sin\theta \ \sin(n+1)\theta} \,,$$

$$Q_{ij} = -\frac{r^{i-j}\sin j\theta\ \sin(n+1-i)\theta}{\sqrt{c_{-1}c_1}\sin\theta\ \sin(n+1)\theta}\,. \tag{17}$$

If $c_1 < 0$, the signs of P and Q should be changed.

As our objective was to give explicit expressions for the inverse, we will show how to avoid evaluating θ and the trigonometric functions above. The Chebyshev polynomials [1] of the first and second kinds are $T_n(x) = \cos n\theta$, $U_n(x) = \sin(n+1)\theta/\sin\theta$, where $x = \cos\theta$; both satisfy the recurrence $T_n = 2xT_{n-1} - T_{n-2}$, the first few terms being $T_0 = 1$, $T_1(x) = x$, $U_0 = 1$, $U_1 = 2x$. Putting $x = \cos\theta = -c_0/2rc_1$, (17) becomes

$$P_{ij} = -r^{i-j}U_{i-1}(x)[T_j(x) - U_{j-1}(x)T_{n+1}(x)/U_n(x)]/\sqrt{c_{-1}c_1}\,,$$

$$Q_{ij} = -r^{i-j}U_{j-1}(x)[T_i(x) - U_{i-1}(x)T_{n+1}(x)/U_n(x)]/\sqrt{c_{-1}c_1}\,.$$

Note in passing that these forms of the inverse agree with Barrett's theorem [6] that A is tridiagonal iff A^{-1} is of the form

$$A^{-1}_{i,j} = \begin{cases} x_iy_j\,, & i \le j \\ u_iv_j\,, & i > j \end{cases}$$

provided $u_iv_i = x_iy_i$, $i = 1, \ldots, n$.

3.2 Example: third order difference operator matrix

Consider the nonsymmetric third order difference operator matrix ($p = 2$, $q = 1$)

$$A = \begin{bmatrix} 3 & -1 & 0 & 0 & \cdots & 0 \\ -3 & 3 & -1 & 0 & \cdots & 0 \\ 1 & -3 & 3 & -1 & & 0 \\ & \ddots & \ddots & \ddots & \ddots & \\ 0 & & 1 & -3 & 3 & -1 \\ 0 & \cdots & 0 & 1 & -3 & 3 \end{bmatrix}$$

The inverse of this matrix is

$$A^{-1}_{ij} = \begin{cases} a_0(j)i(i+1)\,, & i \le j \\ b_0(j)i^2 + b_1(j)i + b_2(j)\,, & i \ge j-1 \end{cases}$$

where

$$\begin{aligned} a_0(j) &= (1-j+n)(2-j+n)/c\,, \\ b_0(j) &= j(-3+j-2n)/c\,, \\ b_1(j) &= j(1+j+4n+2n^2)/c\,, \\ b_2(j) &= -(-1+j)j/2\,, \\ c &= 2(n+1)(n+2)\,. \end{aligned}$$

In this case P and Q are second-order polynomials in i and j, which are equal for $i = j-1, j$.

For example, the first column of A^{-1} is $Q_{i1} = i(n+1-i)/(n+2)$.

Theorem 2 *For $n \ge 1$, the determinant of the third order difference operator matrix A_n is*

$$|A_n| = (n+1)(n+2)/2\,.$$

Proof: Partition A_n as

$$A_{n+1} = \begin{bmatrix} B & C \\ D & A_n \end{bmatrix}$$

where $B = 3\,,\ D' = \begin{bmatrix} -3 & 1 & 0 & 0 & \cdots \end{bmatrix}$ and $C = \begin{bmatrix} -1 & 0 & 0 & \cdots \end{bmatrix}$. Then using the well known result $|A_{n+1}| = |A_n|\,|B - CA_n^{-1}D|$ and the above expression for the inverse, we get

$$CA_n^{-1}D = 2n/(n+1)\,.$$

The proof then follows by induction. ♠

3.3 Example: fourth order difference operator matrix

Consider the symmetric Toeplitz matrix ($p = q = 2$)

$$A = \begin{bmatrix} 6 & -4 & 1 & 0 & \cdots & 0 & 0 \\ -4 & 6 & -4 & 1 & 0 & \cdots & 0 \\ 1 & -4 & 6 & -4 & 1 & & 0 \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & 1 & -4 & 6 & -4 \\ 0 & 0 & \cdots & 0 & 1 & -4 & 6 \end{bmatrix} \tag{18}$$

This matrix was also considered in [2] and [16] using less general methods. We can write down the first column of the inverse of this matrix by inspection: since the solutions to the difference equation (4) in this case are $r(i) = \{1, i, i^2, i^3\}$ and it follows from (7) that $Q_{i1} = 0$ for $i = 0$, $n+1$ and $n+2$ we have

$$Q_{i1} = ci(n+1-i)(n+2-i)$$

and c can be found from $6Q_{11} - 4Q_{21} + Q_{31} = 1$ giving

$$A^{-1}_{i,1} = i\frac{(n+1-i)(n+2-i)}{(n+2)(n+3)} \,.$$

Note that since A is centrosymmetric, having found the first column, we then have the other first and last columns and rows, and we can then use the formula of Trench [32, p207], [11, 31, p188], namely if T_n is a Toeplitz matrix, then putting $T_n^{-1} = (h_{ij})$, provided $h_{00} \neq 0$ we have

$$h_{ij} = h_{i-1,j-1} + (h_{00})^{-1}[h_{i0}h_{0j} - h_{n-j+1,0}h_{0,n-i+1}], \quad 0 \le i,j \le n \,.$$

In full, the inverse of the fourth-order difference operator matrix (18) is

$$A^{-1}_{ij} = \begin{cases} a_0 i^3 + a_1 i^2 + a_2 i \,, & i \le j+1 \\ b_0 i^3 + b_1 i^2 + b_2 i + b_3 \,, & i \ge j-1 \end{cases}$$

where we have dropped the j subscript to improve readability, and

$$\begin{aligned} a_0 &= -(3+2j+n)d_j/c \\ a_1 &= 3j(1+n)d_j/c \\ a_2 &= (3+5j+n+3jn)d_j/c \\ b_0 &= (5-2j+3n)e_j/c \\ b_1 &= -3(1+n)(4-j+2n)e_j/c \\ b_2 &= (1+5j+12n+3jn+12n^2+3n^3)e_j/c \\ b_3 &= (1-j)e_j/6 \end{aligned}$$

and $d_j = (n-j+1)(n-j+2)$, $e_j = j(j+1)$, $c = 6(n+1)(n+2)(n+3)$.

Here P and Q are cubic polynomials in i and j, which are equal for $i = j-1, j, j+1$. The inverse is of course symmetric, so we do not have to derive b_k in this case.

Theorem 3 *For $n \geq 1$, the determinant of the fourth order difference operator matrix A_n is*

$$|A_n| = (n+1)(n+2)^2(n+3)/12\,.$$

Proof: Partition A_n as

$$A_n = \begin{bmatrix} B & D' \\ D & A_{n-1} \end{bmatrix}$$

where $B = 6\,,\quad D' = [\,-4 \quad 1 \quad 0 \quad 0 \quad \cdots\,]$. Then using the well known result $|A_n| = |A_{n-1}|\,|B - D'A_{n-1}^{-1}D|$ and the above expression for the inverse, we get

$$D'A_{n-1}^{-1}D = (5n+6)(n-1)/(n(n+1))\,.$$

The proof then follows by induction. ♠

4 Tridiagonal matrix with modified corner elements

Because many of the above examples had an inverse which was a tridiagonal matrix with constant diagonals except for the corner elements, we will derive the inverse of a matrix of this form.

The method of §3 extends easily to this case, which amounts to a change in the boundary conditions, and we can do the same for any first and last row, but our ansatz (5) will not apply to all A^{-1} if we alter any other rows.

Let

$$A = \begin{bmatrix} d & c_1 & 0 & \dots & 0 & e \\ c_{-1} & c_0 & c_1 & 0 & \dots & 0 \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ 0 & \dots & 0 & c_{-1} & c_0 & c_1 \\ e & 0 & \dots & 0 & c_{-1} & d \end{bmatrix}.$$

In the above notation we have $p = q = 1$, and $r_k(i)$ are two independent solutions of the difference equation $c_{-1}r(i) + c_0 r(i+1) + c_1 r(i+2) = 0$. The inverse is

$$A^{-1}_{ij} = \begin{cases} P_{ij}\,, & 1 \le i \le j \\ Q_{ij}\,, & j \le i \le n \end{cases}$$

where P, Q are as in (5). Proceeding as above we multiply rows $i = 1, j, n$ of A by column j of A^{-1} to get the equations

$$\begin{aligned} dP_{1,j} + c_1 P_{2j} + eQ_{nj} &= 0\,, && (19)\\ -P_{j+1,j} + Q_{j+1,j} &= 1/c_1\,, && (20)\\ eP_{1j} + c_{-1}Q_{n-1,j} + dQ_{nj} &= 0\,, && (21)\\ P_{jj} &= Q_{jj}\,. && (22) \end{aligned}$$

From (20,22) we have again

$$\begin{aligned} z_1(j) &= -r_2(j)/c_1 D(j)\,,\\ z_2(j) &= r_1(j)/c_1 D(j)\,, \end{aligned}$$

as in (15), and (19,21) give

$$\begin{aligned} f_1 a_1(j) + f_2 a_2(j) &= e\sum_k^2 z_k(j) r_k(n)\,,\\ g_1 a_1(j) + g_2 a_2(j) &= \sum_k^2 z_k(j)(c_{-1} r_k(n-1) + d r_k(n))\,, \quad (23) \end{aligned}$$

where

$$f_k = dr_k(1) + c_1 r_k(2) + er_k(n)\,,$$
$$g_k = er_k(1) + c_{-1} r_k(n-1) + dr_k(n)\,.$$

Solving (23) gives a_k and we apply (11) to give the inverse. It is not immediately obvious that (19–22) apply for $j = 1$ and $j = n$; however, by working out these cases separately, they can be shown to conform to the above.

Example: $d = e = 1$, $c = \{-2, 3, -1\}$ we get $r(i) = \{1, 2^i\}$ then

$$A^{-1}_{ij} = \begin{cases} 2^{i-1} - 2^{n-1} + 2^{n-j}\,, & i \le j \\ 2^{i-1} - 2^{n-1} + 2^{n-j} + 1 - 2^{i-j}\,, & i \ge j \end{cases}$$

Comparing this to (15) we see that the inverse still consists of linear combinations and products of 2^i and 2^{-j}. For $n = 8$ this is

$$A^{-1} = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \\ -2 & 3 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2 & 3 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 3 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 & 3 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2 & 3 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2 & 3 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 & -2 & 1 \end{bmatrix}^{-1}$$

$$= \begin{bmatrix} 1 & -63 & -95 & -111 & -119 & -123 & -125 & -126 \\ 1 & -62 & -94 & -110 & -118 & -122 & -124 & -125 \\ 1 & -61 & -92 & -108 & -116 & -120 & -122 & -123 \\ 1 & -59 & -89 & -104 & -112 & -116 & -118 & -119 \\ 1 & -55 & -83 & -97 & -104 & -108 & -110 & -111 \\ 1 & -47 & -71 & -83 & -89 & -92 & -94 & -95 \\ 1 & -31 & -47 & -55 & -59 & -61 & -62 & -63 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

5 Conclusion

We have described fifteen matrices and six examples, some of which are new, and all of which have easily constructible inverses. The hyperbolic, trigonometric and generalized Fiedler matrices are particularly striking. We described a simple method for inverting band Toeplitz matrices, which is extendable to other cases. We gave results for the tridiagonal case, in the hope that these were complete, easily applicable and useful, as whereas many authors quote particular cases, the complete treatment for all cases of the diagonals does not seem to be readily available. One form that recurs is the tridiagonal with modified corner elements, which we inverted.

At the time of publishing, FORTRAN programs which implement the formulae in this paper are available from `http://anusf.anu.edu.au/~mld900/math/toeplitz/`.

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