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Analytical inversion of symmetric tridiagonal matrices

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Abstract. In this paper we present an analytical formula for the inversion of symmetrical tridiagonal matrices. The result is of relevance to the solution of a variety of problems in mathematics and physics. As an example, the formula is used to derive an exact analytical solution for the one-dimensional discrete Poisson equation with Dirichlet boundary conditions.

Many mathematical [1, 2] and physical problems [2, 3] require the inversion of the $k \times k$ symmetric tridiagonal matrices

$$\mathbf{M}_k = \begin{pmatrix} D & 1 & 0 & 0 & \dots & & & & 0 \\ 1 & D & 1 & 0 & \dots & & & & 0 \\ 0 & 1 & D & 1 & \dots & & & & 0 \\ \dots & & & & \dots & & & & \dots \\ & & & & \dots & & & & \\ & & & & \dots & & & & \\ \dots & & & & \dots & & & & \dots \\ 0 & 0 & 0 & & \dots & 1 & D & 1 & 0 \\ 0 & 0 & 0 & & \dots & 0 & 1 & D & 1 \\ 0 & 0 & 0 & & \dots & 0 & 0 & 1 & D \end{pmatrix} \tag{1}$$

where D is an arbitrary constant. To our knowledge, in the literature [1, 2] the inversion of (1) is carried out either by numerical means or by the eigenvalue method. In this short paper, we present an analytical form for the inversion of matrix (1).

Our way of obtaining the inverse matrix for the tridiagonal matrix $\mathbf{M}_k$ as given by (1), is to calculate directly its determinant $M_k = \det(\mathbf{M}_k)$ and co-factor $A_{ij} = \mathrm{cof}(M_{ij})$. The value of the determinant M_k can be evaluated analytically in the following way. First, it is straightforward to show that there is a special recursion relation between the consecutive M_k given by

$$M_{i+1} = DM_i - M_{i-1} \tag{2}$$

with the boundary conditions

$$M_0 = 1 \qquad M_1 = D. \tag{3}$$

To solve for equations (2) and (3), we seek a series solution,

$$M_k = \sum_{j=1}^{k} a_j D^j. \tag{4}$$

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After some direct algebra, we obtain

$$M_k = \sum_{i=0}^{[k/2]} (-1)^i \binom{k-i}{i} D^{k-2i} \tag{5}$$

where $[x]$ is the integer part of x.

If $D \leqslant -2$ (of interest in the analysis of various physical systems [1–3]), it is convenient to let $D = -2\cosh\lambda$. Then, using a well known formula from [4], we reduce (5) to the form

$$M_k = (-1)^k \sinh(k+1)\lambda / \sinh\lambda \tag{6}$$

where λ is given by

$$D = -2\cosh\lambda. \tag{7}$$

When $D \geqslant 2$, we let $D = 2\cosh\lambda$, and find that M_k can again be written in the same form as in (6) except for the omission of the $(-1)^k$ factor. Finally, for $-2 < D < 2$, we let $D = 2\cos\lambda$, and then M_k takes the same form as in (6) except that the hyperbolic sines in (6) are replaced by sines.

Next, we solve for the co-factor A_{ij} of (1). Because of the special structure of the tridiagonal matrix $\mathbf{M}_k$ as seen in (1), its co-factor A_{ij} can be evaluated conveniently based on the following observations. One notices that whenever the ith row and the jth column in the determinant M_k is struck out, it becomes a determinant of order $(k-1)\times(k-1)$ having three decoupled sub-blocks with the order of $(i-1)$, $(k-j)$, and $(j-i)$, respectively (here we have assumed $j > i$, the $i > j$ case can be addressed in a similar fashion). The $(i-1)$ and $(k-j)$ sub-blocks possess the original tridiagonal form of M_k, while the $(j-i)$ sub-block is uptriangular with unit diagonal elements and has unit determinant value. It follows that the value of the co-factor A_{ij}, which is the product of $(-1)^{i+j}$ with the determinants of the above mentioned three sub-blocks, takes the form of

$$A_{ij} = (-1)^{i+j} M_{i-1} M_{k-j-1} \qquad \text{for } i < j \tag{8}$$

and it is symmetric with respect to the interchange of i and j.

By definition, the elements of the inverse matrix of a k by k matrix $\mathbf{M}_k$ is given by $R_{ij} = A_{ji}/M_k$. Using (8), we obtain

$$R_{ij} = (-1)^{i+j} M_{i-1} M_{k-j} / M_k \qquad \text{for } i < j \tag{9}$$

and it is symmetric with respect to the interchange of i and j.

For $D \leqslant -2$, we substitute (6) into (9) and obtain an analytical expression for the elements of the inverse matrices $\mathbf{R}_k$ for the matrices (1) as

$$R_{ij} = -\frac{\cosh(k+1-|j-i|)\lambda - \cosh(k+1-i-j)\lambda}{2\sinh\lambda\sinh(k+1)\lambda}. \tag{10}$$

For $D \geqslant 2$, the elements of the inverse matrix for (1) have the same form as (10), except that the minus sign on the right-hand side is replaced by $(-1)^{i+j}$. Also, for $-2 < D < 2$, the hyperbolic sines and cosines in (10) becomes sines and cosines, respectively.

Equation (10) should be useful in obtaining solutions of many physical problems. In particular, we mention our work on various single-charge-tunnelling systems where this result proved invaluable [3]. As an another example, we use (10) to solve the following finite difference equation associated with the one-dimensional Poisson equation with Dirichlet boundary conditions [1, 2],

$$\mathbf{M}\bar{\varphi} = \bar{\rho} \tag{11}$$

where $\bar{\varphi}$ is the discrete potential column, $\bar{\rho}$ is the column related to the source, and the k by k matrix $\mathbf{M}$ takes the form of (1) with $D = -2$. It follows from (7) that $\lambda = 0$. Thus, in terms of (10), the solution of (11) can be written as

$$\bar{\varphi} = \mathbf{M}^{-1}\bar{\rho} \equiv \mathbf{R}\bar{\rho} \tag{12}$$

where

$$R_{ij} = -\frac{(i + j - |j - i|)(2k + 2 - |j - i| - i - j)}{4(k + 1)}. \tag{13}$$

In summary, in this paper we have presented an analytical form (10) for the inversion of the symmetrical tridiagonal matrices (1). The formula has been used to derive an exact analytical solution (13) for the one-dimensional discrete Poisson equation (11) with Dirichlet boundary conditions. It is also clear that the result is of relevance to the solution of a variety of problems in mathematics and physics.

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