The analytic inversion of any finite symmetric tridiagonal matrix

1997 J. Phys. A: Math. Gen. 30 2889

(http://iopscience.iop.org/0305-4470/30/8/029)

J. Phys. A: Math. Gen. **30** (1997) 2889–2893. Printed in the UK PII: S0305-4470(97)77256-1

COMMENT

The analytic inversion of any finite symmetric tridiagonal matrix

H A Yamani†‡ and M S Abdelmonem§

† Ministry of Industry and Electricity, PO Box 56729, Riyadh 11127, Saudi Arabia

‡ Physics Department, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

§ Energy Resources Division, Research Institute, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

Received 19 August 1996, in final form 6 November 1996

Abstract. We use the theory of orthogonal polynomials to write down explicit expressions for the polynomials of the first and second kind associated with a given infinite symmetric tridagonal matrix H. The Green's function is the inverse of the infinite symmetric tridiagonal matrix $(H - zI)$. By calculating the inverse of the finite symmetric tridiagonal matrix $(H_{PP} - zI_{PP})$ we can find the analytical form of the inverse of the finite symmetric tridiagonal matrix, H_{PP}.

The matrix representation of many physical operators are tridiagonal in a certain basis set. In fact some computational methods, such as the recursion [1–3] and Lanczos [4] methods, are based on the scheme of creating a basis that renders a given system Hamiltonian operator H tridiagonal. The advantage of this representation lies in the intimate connection between tridiagonal matrices and the theories of orthogonal polynomials, continued fractions, and the quadrature approximation [5]. This connection is exploited to invert the tridiagonal matrix by generally finding the matrix representation of the Green functions.

This comment is motivated by the recent work of Hu and O'Connell [6] who solved for the inverse of a simple tridiagonal matrix with entries of a constant D along the diagonal and with unity along the off-diagonal. Here we show that it is simple to generalize their work by using the theory of orthogonal polynomials to invert a given finite symmetric tridiagonal matrix whose diagonal and off-diagonal elements have general values. We start by considering the case of the infinite symmetric tridiagonal matrix, H. By using the theory of orthogonal polynomials, we define two sets of polynomials $\{p_n(z)\}_{n=0}^{\infty}$ and $\{q_n(z)\}_{n=0}^{\infty}$, which we call the polynomials of the first and second kind, associated with the infinite matrix, H. The Green function, $G(z)$, is the inverse of the infinite matrix $(H - zI)$, where I is the infinite unit matrix. The element $G_{nm}(z)$ can be written in terms of p and q. $G(0)$ is of course the inverse of the infinite matrix H. In a similar fashion, we find the inverse of the symmetric tridiagonal matrix $(H_{PP} - zI_{PP})$ of rank N. Here, I_{PP} is the unit matrix of rank N. Consequently, we find the analytical form of the inverse of the finite matrix H_{PP}.

To proceed, we first review the results derivable from the theory of orthogonal polynomials [7]. We consider an infinite symmetric tridiagonal matrix H given by

$$H_{nm} = \begin{cases} a_n & \text{if } m = n \\ b_n & \text{if } m = n+1 \end{cases} \tag{1}$$

where $n, m = 0, 1, 2, \ldots$. We assume that all the a_n are real and all the b_n are positive. It is known from the theory of orthogonal polynomials [7] that associated with this tridiagonal matrix are two sets of polynomials $\{p_n(z)\}_{n=0}^{\infty}$ and $\{q_n(z)\}_{n=0}^{\infty}$ defined, for any complex z, by

$$\begin{aligned} &p_0(z) = 1 \qquad \text{and} \qquad p_1(z) = (z - a_0)/b_0 \\ &q_0(z) = 0 \qquad \text{and} \qquad q_1(z) = 1/b_0 \end{aligned} \tag{2}$$

and both satisfy the three-term recursion relation

$$zs_n(z) = b_{n-1}s_{n-1}(z) + a_n s_n(z) + b_n s_{n+1}(z) \qquad n \geqslant 1 \tag{3}$$

where $s_n(z)$ may stand for either $p_n(z)$ or $q_n(z)$. We note that $p_n(z)$ is a polynomial of order n in z and we call it polynomial of the first kind. Also, $q_n(z)$ is a polynomial of order $(n-1)$ in z and we call it a polynomial of the second kind. Both polynomials satisfy the Wronskian-like relation

$$b_k\{p_k(z)q_{k+1}(z) - p_{k+1}(z)q_k(z)\} = 1 \qquad k \geqslant 0. \tag{4}$$

The ratio $[q_n(z)/p_n(z)]$ has the continued-fraction representation [1–3]

$$\left[\frac{q_n(z)}{p_n(z)}\right] = \frac{1}{(z-a_0)-}\,\frac{b_0^2}{(z-a_1)-}\,\frac{b_1^2}{(z-a_2)-\cdots}\,\frac{b_{n-3}^2}{(z-a_{n-2})-}\,\frac{b_{n-2}^2}{(z-a_{n-1})}. \tag{5}$$

The Green function $G(z)$ associated with the matrix H is defined by the relation

$$(H - zI)G(z) = I. \tag{6}$$

The matrix element $G_{nm}(z)$ can be written in terms of $G_{00}(z)$ and the polynomials $p_n(z)$ and $q_n(z)$ as follows [7],

$$G_{nm}(z) = p_n(z)p_m(z)\left\{G_{00}(z) + \frac{q_{n_>}(z)}{p_{n_>}(z)}\right\} \tag{7}$$

where $n_>$ is the larger of n and m. The element $G_{00}(z)$ has a particularly simple continued-fraction representation [7]

$$G_{00}(z) = -\lim_{n\to\infty}\left(\frac{q_n(z)}{p_n(z)}\right). \tag{8}$$

We note that $G(0)$ is the inverse of the infinite symmetric tridiagonal matrix H.

We now proceed to find the analytical form of the inverse of a finite symmetric tridiagonal matrix, H_{PP}, of rank N. We partition the infinite matrix H into a finite P-part of dimension N and an infinite Q-part as

$$H = \begin{pmatrix} H_{PP} & H_{PQ} \\ H_{QP} & H_{QQ} \end{pmatrix} \tag{9}$$

where H_{PP} has the matrix representation

$$H_{PP} \sim \begin{pmatrix} a_0 & b_0 & 0 & 0 & \ldots & 0 & 0 & 0 \\ b_0 & a_1 & b_1 & 0 & \ldots & 0 & 0 & 0 \\ 0 & b_1 & a_2 & b_2 & \ldots & 0 & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & 0 & \ldots & b_{N-3} & a_{N-2} & b_{N-2} \\ 0 & 0 & 0 & 0 & \ldots & 0 & b_{N-2} & a_{N-1} \end{pmatrix} \tag{10}$$

and H_{QQ} has the infinite matrix representation

$$(H_{QQ})_{nm} = (H)_{n+N,m+N}. \tag{11}$$

We propose to calculate the inverse of the finite matrix H_{PP}. We find it more convenient to calculate the inverse of the matrix $(H_{PP} - zI_{PP})$.

We know that

$$\begin{pmatrix} (H_{PP} - zI_{PP}) & H_{PQ} \\ H_{QP} & (H_{QQ} - zI_{QQ}) \end{pmatrix} \begin{pmatrix} G_{PP} & G_{PQ} \\ G_{QP} & G_{QQ} \end{pmatrix} - \begin{pmatrix} I_{PP} & 0 \\ 0 & I_{QQ} \end{pmatrix}. \tag{12}$$

One of these equations gives

$$(H_{PP} - zI_{PP})G_{PP} + H_{PQ}G_{QP} = I_{PP}. \tag{13}$$

Thus

$$(H_{PP} - zI_{PP})^{-1} = G_{PP}(I_{PP} - H_{PQ}G_{QP})^{-1}. \tag{14}$$

Now the finite matrix $(I_{PP} - H_{PQ}G_{QP})$ is a simple looking $N \times N$ matrix, due to the fact that H_{PQ} has only one non-vanishing element. More explicitly

$$(I_{PP} - H_{PQ}G_{QP})_{ij} = \delta_{ij} - H_{N-1,N}G_{N,j}\delta_{i,N-1}. \tag{15}$$

To invert this matrix, we define

$$K_{PP} = (I_{PP} - H_{PQ}G_{QP})\left(I_{PP} + \frac{1}{\Delta}H_{PQ}G_{QP}\right) \tag{16}$$

where

$$\begin{aligned} \Delta &= 1 - b_{N-1}G_{N,N-1}(z) \\ &= 1 - b_{N-1}p_N(z)p_{N-1}(z)\left(G_{00}(z) + \frac{q_N(z)}{p_N(z)}\right). \end{aligned} \tag{17}$$

Now

$$\begin{aligned} (K_{PP})_{i,j} = \delta_{i,j} &- \delta_{i,N-1}H_{N-1,N}G_{N,j} + \frac{1}{\Delta}\delta_{i,N-1}H_{N-1,N}G_{N-1,j} \\ &- \frac{1}{\Delta}\delta_{i,N-1}H_{N-1,N}G_{N,N-1}H_{N-1,N}G_{N-1,j}. \end{aligned} \tag{18}$$

With an explicit form for Δ of equation (17), we can easily show that the last three terms in equation (18) vanish. Thus

$$(K_{PP})_{i,j} = \delta_{i,j}. \tag{19}$$

Therefore,

$$(I_{PP} - H_{PQ}G_{QP})^{-1} = \left(I_{PP} + \frac{1}{\Delta}H_{PQ}G_{QP}\right). \tag{20}$$

Furthermore, by using the Wronskian-like relation (4), we can show that Δ has the following alternative form:

$$\Delta = -b_{N-1}p_N(z)p_{N-1}(z)\left(G_{00}(z) + \frac{q_{N-1}(z)}{p_{N-1}(z)}\right). \tag{21}$$

From equations (14) and (21) and assuming $j \geqslant i$, we may write

$$\begin{aligned} [(H_{PP} - zI_{PP})^{-1}]_{ij} &= \left[G_{PP}\left(I_{PP} + \frac{1}{\Delta}H_{PQ}G_{QP}\right)\right]_{i,j} \\ &= \frac{1}{\Delta}[G_{ij}\Delta + G_{i,N-1}b_{N-1}G_{N,j}]. \end{aligned} \tag{22}$$

Substituting explicitly for the various Green function matrix elements, we finally obtain

$$[(H_{PP} - zI_{PP})^{-1}]_{i,j} = \left[\frac{q_j(z)}{p_j(z)} - \frac{q_N(z)}{p_N(z)}\right] p_i(z) p_j(z) \qquad \text{for } N-1 \geqslant j \geqslant i \geqslant 0. \tag{23}$$

This matrix is of course symmetric. It is to be noted that the analytical form equation (23) of the inverse of the finite symmetric tridiagonal matrix $(H_{PP} - zI_{PP})$ depends totally on p and q which can be calculated easily using equations (2), (3) and (5) in terms of the sets $\{a_n\}_{n=0}^{N-1}$ and $\{b_n\}_{n=0}^{N-2}$. Finally, the inverse of H_{PP} is obtained from equation (23) by setting $z = 0$.

To show that our results reduce to those of Hu and O'Connell [6], we consider the case $-2 < D < 2$. The other cases can be treated similarly. Equation (23) can be written as

$$[(H_{PP} - zI_{PP})^{-1}]_{ij} = -[q_N(z)p_j(z) - p_N(z)q_j(z)]\frac{p_i(z)}{p_N(z)} \qquad \text{for } N-1 \geqslant j \geqslant i \geqslant 0. \tag{24}$$

We define

$$Q_j(z) = q_N(z)p_{N-j}(z) - q_{N-j}(z)p_N(z) \tag{25}$$

and can easily show that

$$B_{j-1}Q_{j-1}(z) + A_j Q_j(z) + B_j Q_{j+1}(z) = zQ_j(z) \tag{26}$$

where $A_j = a_{N-j}$ and $B_j = b_{N-j-1}$. Furthermore, $Q_0(z) = 0$ and $Q_1(z) = 1/b_{N-1} = 1/B_0$. Thus $Q_j(z)$ can be generated in exactly the same way as $q_j(z)$ except that A_j replaces a_j and B_j replaces b_j. Now since in our case $a_j = D$ and $b_j = 1$ where D is a constant, we immediately conclude that

$$Q_j(z) = q_j(z). \tag{27}$$

Thus,

$$[(H_{PP} - zI_{PP})^{-1}]_{ij} = -q_{N-j}(z)\frac{p_i(z)}{p_N(z)} \qquad \text{for } N-1 \geqslant j \geqslant i \geqslant 0. \tag{28}$$

Setting $z = 0$, we have

$$[(H_{PP})^{-1}]_{ij} = -q_{N-j}(0)\frac{p_i(0)}{p_N(0)}. \tag{29}$$

Except for the initial conditions both $p_i(0)$ and $q_i(0)$ satisfy the recursion relation (3), namely

$$0 = s_{j-1}(0) + Ds_j(0) + s_{j+1}(0). \tag{30}$$

Now, writing $D = 2x$ and $x = \cos\lambda$ we have

$$-2xs_j(0) = s_{j-1}(0) + s_{j+1}(0). \tag{31}$$

Except for the minus sign on the left-hand side of this equation, this is just the three-term recursion relation satisfied by the Chebychev polynomials of the first kind

$$T_j(x) = \cos(j\lambda) \tag{32}$$

and the Chebychev polynomials of the second kind

$$U_j(x) = \frac{\sin(j+1)\lambda}{\sin\lambda}. \tag{33}$$

It is easy to show that, due to the initial condition of $p_i(0)$ and $q_i(0)$, we have

$$p_j(0) = (-1)^j U_j(x)$$

and

$$q_j(0) = \frac{(-1)^{j-1}}{x}(U_j(x) - T_j(x)) = (-1)^{j-1}\frac{\sin j\lambda}{\sin\lambda} = (-1)^{j-1}U_{j-1}(x). \quad (34)$$

Therefore,

$$[(H_{PP})^{-1}]_{ij} = (-1)^{j-1}U_{N-j}(x)\frac{U_i(x)}{U_N(x)} = (-1)^{j-1}\frac{\sin(N-j)\lambda}{\sin\lambda}\frac{\sin(i+1)\lambda}{\sin(N+1)\lambda}$$
$$= (-1)^{j-1}\frac{[\cos(N-1-j-i)\lambda - \cos(N+1-j+i)\lambda]}{2\sin\lambda\sin(N+1)\lambda}. \quad (35)$$

This result is the same as that of Hu and O'Connell [6] since our indices i and j range from 0 to $(N-1)$ while theirs range from 1 to N.

Acknowledgment

The support of this work by the Research Institute is gratefully acknowledged.

References

[1] Bullett D, Haydock R, Heine V and Kelly M J 1980 *Solid State Physics* vol 35 (New York: Academic)
[2] Haydock R, Heine V and Kelly M J 1972 *J. Phys.: Condens. Matter* **5** 2845
[3] Pettifor D G and Weaire D L (eds) 1985 *The Recursion Method and its Applications* (Berlin: Springer)
[4] Lanczos C 1950 *J. Res. Nat. Bur. Stand.* **45** 255
[5] Haymaker R W and Schlessinger L 1970 *The Padé Approximants in Theoretical Physics* ed G A Baker and J L Gammel (New York: Academic)
[6] Hu G Y and O'Connell R F 1996 *J. Phys. A: Math. Gen.* **29** 1511
[7] Akhiezer N I 1965 *The Classical Moment Problem* (Edinburgh: Oliver and Boyd)