Series solution of certain Sturm–Liouville eigenvalue problems

By D. J. Green* and S. Michaelson†

The solutions of certain Sturm–Liouville eigenvalue problems are known in the form of orthogonal functions $\phi_r(x)$, $r = 0, 1, 2, \ldots$, arranged so that the moduli of the corresponding eigenvalues λ_r increase monotonically with r, i.e.

$$\mathscr{L}\phi_r(x) = \lambda_r \rho(x)\phi_r(x)$$

with the $\phi_r(x)$ satisfying appropriate boundary conditions.

The investigations described in this paper are an attempt to examine the conditions that must be satisfied in order that the extended eigenvalue problem

$$\mathscr{L}U + q(x)U = \mu\rho(x)U$$

(again with U satisfying appropriate boundary conditions) may be solved by expansion of U in a series of the orthogonal functions $\phi_r(x)$.

Practically all orthogonal systems satisfy a 3-term recurrence relation. If the $\phi_r(x)$ satisfy such a relation, this, together with the differential equations satisfied by the $\phi_r(x)$, may be used to transform the extended differential eigenvalue problem to that of finding the eigenvalues of an infinite symmetric tri-diagonal matrix. An examination is made of the recurrence relations satisfied by the ortho-normal polynomials, and the conditions that must be satisfied by the coefficients of the basic recursion in order that certain polynomial operators may give such matrices are obtained. The results are applied to the Jacobi polynomials and Fourier functions.

A discussion of the convergence of the eigenvalues obtained by repeatedly bordering finite principal submatrices of the infinite matrices follows. Several numerical examples are given, the calculations being made on the University of London Ferranti Mercury computer.

1. Introduction

The general Sturm–Liouville problem is that of finding non-trivial functions $U_i(x)$, and corresponding parameters λ_i, which satisfy the differential equation

$$\mathscr{L}U = \frac{d}{dx}\left\{p(x)\frac{dU}{dx}\right\} + q_1(x)U = \lambda\rho(x)U \quad (1.1)$$

in the range (a, b), and boundary conditions which result in

$$[p(x)(U_jU_i' - U_iU_j')]_a^b = 0 \quad \text{for} \quad i \neq j \quad (1.2)$$

where the dash indicates differentiation with respect to x.

The boundary conditions can take a variety of forms. For example, if $p(a) \neq 0$ and $p(b) \neq 0$, homogeneous boundary conditions

$$\left.\begin{aligned} \alpha' U_i(a) + \alpha U_i'(a) = 0 \\ \beta' U_i(b) + \beta U_i'(b) = 0 \end{aligned}\right\} \quad (1.3)$$

where neither both the constants α and α' nor both the constants β and β' are zero, may be required. Alternatively, if $p(a) = p(b) = 0$, U_i and U_i' must remain bounded at both $x = a$ and $x = b$.

Lanczos (1950) has suggested a method by which the analytical solution of the general problem may be obtained. His technique, however, involves finding the Green's function $K(x, t)$ of the operator $\mathscr{L}$. This is available in closed form in comparatively few cases. Further, the iteration process requires repeated integrations which may go beyond our analytical facilities.

The solution of certain problems has been obtained in the form of orthogonal functions $\phi_r(x)$, $r = 0, 1, 2, \ldots$, arranged so that the moduli of the corresponding eigenvalues λ_r increase monotonically with r, i.e.

$$\mathscr{L}\phi_r(x) = \lambda_r\rho(x)\phi_r(x). \quad (1.4)$$

The purpose of this investigation is to examine the conditions that must be satisfied so that the extended eigenvalue problem

$$\mathscr{L}U + q_2(x)\rho(x)U = \mu\rho(x)U \quad (1.5)$$

(with the same boundary conditions as those associated with the operator $\mathscr{L}$) may be solved by expansion of U in a series of the orthogonal functions $\phi_r(x)$.

It will be shown that for certain operators the problem (1.5) can be reduced to finding the eigenvalues of an infinite symmetrical tri-diagonal matrix. For some of these matrices the sequences formed of corresponding eigenvalues of finite leading principal sub-matrices are very convergent.

2. Reduction to tri-diagonal form

Suppose the $\phi_r(x)$ are ortho-normal functions, being solutions of the eigenvalue problem

$$\mathscr{L}U = \lambda\rho(x)U \quad (2.1)$$

in (a, b) with appropriate boundary conditions.

For such functions

$$\int_a^b \rho(x)\phi_p(x)\phi_q(x)dx = \delta_{pq} \quad (2.2)$$

* *Glamorgan College of Technology, Treforest, Glamorgan.*
† *Edinburgh University Computer Unit*, 7, *Buccleuch Place, Edinburgh* 8.

where δ_{pq} is "Kronecker's symbol";

$$\delta_{pq} = 1 \quad (p = q)$$
$$= 0 \quad (p \neq q).$$

Assume a solution of (1.5) of the form

$$U = \sum_{r=0}^{\infty} \alpha_r \phi_{kr+n}(x) \qquad (2.3)$$

where k is a positive and n a non-negative integer. If

$$U_1 = \sum_{r=0}^{\infty} \alpha_r^{(1)} \phi_{kr+n}(x) \qquad (2.4)$$

$$U_2 = \sum_{r=0}^{\infty} \alpha_r^{(2)} \phi_{kr+n}(x) \qquad (2.5)$$

are two solutions corresponding to the distinct eigenvalues $\lambda = \mu_1$ and $\lambda = \mu_2$ respectively, then

$$\int_a^b \rho(x) \sum_{r=0}^{\infty} \alpha_r^{(1)} \phi_{kr+n}(x) \sum_{r=0}^{\infty} \alpha_r^{(2)} \phi_{kr+n}(x) dx = 0$$

$$\therefore \qquad \sum_{r=0}^{\infty} \alpha_r^{(1)} \alpha_r^{(2)} = 0 \qquad (2.6)$$

i.e. the $\alpha_r^{(i)}$ are orthogonal vectors.

For orthogonal functions (and especially orthogonal polynomials) recurrence relations of the form

$$q_2(x)\phi_n = A_n \phi_{k+n} + B_n \phi_n$$
$$q_2(x)\phi_{kr+n} = A_{kr+n}\phi_{k(r+1)+n} + B_{kr+n}\phi_{kr+n} + C_{kr+n}\phi_{k(r-1)+n}$$
$$r = 1, 2, 3, \ldots \qquad (2.7)$$

where the A_p, B_p, and C_p are independent of x, exist for certain $q_2(x)$.

In fact if the orthogonal functions are normalized, the recurrence relations (2.7) are symmetric and take the form

$$q_2(x)\phi_n = A_n \phi_{k+n} + B_n \phi_n$$
$$q_2(x)\phi_{kr+n} = A_{kr+n}\phi_{k(r+1)+n} + B_{kr+n}\phi_{kr+n} + A_{k(r-1)+n}\phi_{k(r-1)+n}$$
$$r = 1, 2, 3, \ldots \qquad (2.8)$$

The substitution of (2.3) into (1.5) and the application of relations (2.1) and (2.8) gives

$$\rho(x) \sum_{r=0}^{\infty} \alpha_r \lambda_{kr+n}\phi_{kr+n} + \rho(x) \sum_{r=0}^{\infty} \alpha_r (A_{kr+n}\phi_{k(r+1)+n} + B_{kr+n}\phi_{kr+n} + A_{k(r-1)+n}\phi_{k(r-1)+n}) = \mu\rho(x) \sum_{r=0}^{\infty} \alpha_r \phi_{kr+n}.$$

Equating the coefficients of ϕ_{kr+n} leads to the infinite tri-diagonal matrix eigenvalue problem

$$(\lambda_n + B_n)\alpha_0 + A_n\alpha_1 = \mu\alpha_0$$
$$A_{k(r-1)+n}\alpha_{r-1} + (\lambda_{kr+n} + B_{kr+n})\alpha_r + A_{kr+n}\alpha_{r+1} = \mu\alpha_r$$
$$r = 1, 2, 3, \ldots$$

i.e. the problem of finding the eigenvalues of the infinite symmetric tri-diagonal matrix

$$\begin{bmatrix} \lambda_n + B_n & A_n & & & & \\ A_n & \lambda_{k+n} + B_{k+n} & A_{k+n} & & & \\ & \text{—} & \text{—} & \text{—} & & \\ & & & A_{k(r-1)+n} & \lambda_{kr+n} + B_{kr+n} & A_{kr+n} \\ & & & & \text{—} & \text{—} \end{bmatrix} \qquad (2.9)$$

If series (2.3) is truncated at $r = m$, and substituted in (1.5), a finite square segment of the infinite matrix (2.9) is obtained. It will be shown in Section 6 that if the eigenvalues of this finite segment are calculated, and the process repeated with $r = m + 1$, $m + 2, \ldots$, then the sequence of values obtained for corresponding eigenvalues converges very rapidly for certain operators.

3. Orthogonal polynomials

The first class of orthogonal functions considered is the orthogonal polynomials. [See, for example, Jackson (1941) and Szegö (1939).] These satisfy, when normalized, recurrence relations of the form

$$x\phi_0 = a_0\phi_1 + b_0\phi_0$$
$$x\phi_p = a_p\phi_{p+1} + b_p\phi_p + a_{p-1}\phi_{p-1}$$
$$p = 1, 2, 3, \ldots \qquad (3.1)$$

where ϕ_p is a polynomial of precise degree p.

The problem of what operators $q_2(x)$ will give [using (3.1)] recurrence relations of the form (2.8) and hence a symmetric tri-diagonal matrix eigenvalue problem is now considered. In this connection it should be noted that the addition of a constant to $q_2(x)$ merely changes the eigenvalue μ by that constant, and so is omitted in the discussion.

(*a*) $q_2(x) = \beta_1 x$

$$q_2(x)\phi_0 = \beta_1(a_0\phi_1 + b_0\phi_0)$$
$$q_2(x)\phi_p = \beta_1(a_p\phi_{p+1} + b_p\phi_p + a_{p-1}\phi_{p-1})$$
$$p = 1, 2, 3, \ldots \qquad (3.2)$$

This is of the form (2.8) with $k = 1$, $n = 0$.

Thus the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r \phi_r(x) \tag{3.3}$$

will transform

$$\mathscr{L}U + \beta_1 x\rho(x)U = \mu\rho(x)U \tag{3.4}$$

to an eigenvalue problem of type (2.9).

(*b*) $q_2(x) = \beta_2 x^2 + \beta_1 x$

$$\begin{aligned} q_2(x)\phi_p = {} & \beta_2 a_p a_{p+1}\phi_{p+2} + a_p\{(b_{p+1}+b_p)\beta_2 + \beta_1\}\phi_{p+1} \\ & + \{(a_p^2 + b_p^2 + a_{p-1}^2)\beta_2 + \beta_1 b_p\}\phi_p \\ & + a_{p-1}\{(b_p + b_{p-1})\beta_2 + \beta_1\}\phi_{p-1} \\ & + \beta_2 a_{p-1}a_{p-2}\phi_{p-2} \\ & p = 0, 1, 2, \ldots \end{aligned} \tag{3.5}$$

where $a_s = \phi_s = 0$ when s is a negative integer.

There are two ways in which (3.5) can reduce to (2.8). Clearly $k = 2$, but n can be zero or unity.

For $n = 0$ the following set of equations has to be satisfied

$$b_p + b_{p+1} = -\beta_1/\beta_2 \qquad p = 0, 1, 2, \ldots \tag{3.6}$$

Thus if condition (3.6) is satisfied the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r \phi_{2r}(x)$$

will transform

$$\mathscr{L}U + (\beta_2 x^2 + \beta_1 x)\rho(x)U = \mu\rho(x)U \tag{3.7}$$

into a matrix eigenvalue problem of type (2.9).

For $n = 1$ the conditions to be satisfied are identical with those for $n = 0$, and the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r \phi_{2r+1}(x) \tag{3.8}$$

will also convert (3.7) to an eigenvalue problem of type (2.9).

(*c*) $q_2(x) = \beta_3 x^3 + \beta_2 x^2 + \beta_1 x$

$$\begin{aligned} q_2(x)\phi_p = {} & \beta_3 a_p a_{p+1} a_{p+2}\phi_{p+3} + a_p a_{p+1} \\ & \{\beta_3(b_{p+2} + b_{p+1} + b_p) + \beta_2\}\phi_{p+2} \\ & + a_p\{\beta_3(a_{p+1}^2 + b_{p+1}(b_{p+1} + b_p) \\ & + a_p^2 + b_p^2 + a_{p-1}^2) + \beta_2(b_{p+1} + b_p) + \beta_1\}\phi_{p+1} \\ & + \{\beta_3(a_p^2(b_{p+1} + b_p) + b_p(a_p^2 + b_p^2 + a_{p-1}^2) \\ & + a_{p-1}^2(b_p + b_{p-1})) + \beta_2(a_p^2 + b_p^2 + a_{p-1}^2) \\ & + \beta_1 b_p\}\phi_p + a_{p-1}\{\beta_3(a_p^2 + b_p^2 + a_{p-1}^2 \\ & + b_{p-1}(b_p + b_{p-1}) + a_{p-2}^2) \\ & + \beta_2(b_p + b_{p-1}) + \beta_1\}\phi_{p-1} \\ & + a_{p-1}a_{p-2}\{\beta_3(b_p + b_{p-1} + b_{p-2}) \\ & + \beta_2\}\phi_{p-2} + \beta_3 a_{p-1}a_{p-2}a_{p-3}\phi_{p-3} \\ & p = 0, 1, 2, \ldots \end{aligned} \tag{3.9}$$

where $a_s = \phi_s = 0$ when s *is* a negative integer.

Clearly if (3.9) is to reduce to a recurrence relation similar to (2.8) then $k = 3$, and possible values of n are 0, 1, and 2.

For the appropriate terms of (3.9) to vanish

$$\begin{cases} \beta_3(b_{p+2} + b_{p+1} + b_p) + \beta_2 = 0 \\ \beta_3(b_p + b_{p-1} + b_{p-2}) + \beta_2 = 0 \end{cases} \tag{3.10}$$

$$\begin{cases} \beta_3\{a_{p+1}^2 + a_p^2 + a_{p-1}^2 + b_p^2 + b_{p+1}(b_{p+1} + b_p)\} \\ \qquad + \beta_2(b_{p+1} + b_p) + \beta_1 = 0 \\ \beta_3\{a_p^2 + a_{p-1}^2 + a_{p-2}^2 + b_p^2 + b_{p-1}(b_{p-1} + b_p)\} \\ \qquad + \beta_2(b_p + b_{p-1}) + \beta_1 = 0 \end{cases}$$

$$p = n + 3, n + 6, n + 9, \ldots \tag{3.11}$$

and, in addition to (3.10) and (3.11)

For $n = 0$

$$\left.\begin{aligned} & \beta_3(b_2 + b_1 + b_0) + \beta_2 = 0 \\ & \beta_3\{a_1^2 + a_0^2 + b_0^2 + b_1(b_1 + b_0)\} \\ & \qquad + \beta_2(b_1 + b_0) + \beta_1 = 0 \end{aligned}\right\} \tag{3.12}$$

For $n = 1$

$$\left.\begin{aligned} & \beta_3(b_3 + b_2 + b_1) + \beta_1 = 0 \\ & \beta_3[a_2^2 + b_2(b_2 + b_1) + a_1^2 + b_1^2 + a_0^2] \\ & \qquad + \beta_2(b_2 + b_1) + \beta_1 = 0 \\ & \beta_3[a_1^2 + a_0^2 + b_1^2 + b_0(b_1 + b_0)] \\ & \qquad + \beta_2(b_1 + b_0) + \beta_1 = 0 \end{aligned}\right\} \tag{3.13}$$

For $n = 2$

$$\left.\begin{aligned} & \beta_3(b_4 + b_3 + b_2) + \beta_2 = 0 \\ & \beta_3[a_3^2 + a_2^2 + a_1^2 + b_3(b_3 + b_2) + b_2^2] \\ & \qquad + \beta_2(b_3 + b_2) + \beta_1 = 0 \\ & \beta_3[a_2^2 + a_1^2 + a_0^2 + b_1(b_2 + b_1) + b_2^2] \\ & \qquad + \beta_2(b_2 + b_1) + \beta_1 = 0 \\ & \beta_3(b_2 + b_1 + b_0) + \beta_2 = 0 \end{aligned}\right\} \tag{3.14}$$

These conditions simplify in special cases.

For $n = 0$

Taking all the b_p to be equal, and the a_p to be equal for $p = 1, 2, 3, \ldots$ reduces the equations to be satisfied to

$$\left.\begin{aligned} & b_p = -\beta_2/3\beta_3 && p = 0, 1, 2, \ldots \\ & a_p^2 = a_0^2/2 && p = 0, 1, 2, \ldots \\ & a_0^2 = 2(\beta_2^2/3\beta_3^2 - \beta_1/\beta_3)/3. && \end{aligned}\right\} \tag{3.15}$$

For $n = 2$

Again taking all the b_p to be equal, the a_p to be equal for $p = 3, 4, 5, \ldots$, and $a_1 = a_2$ reduces the equations to be satisfied to

$$\left.\begin{aligned} & b_p = -\beta_2/3\beta_3 \\ & a_p^2 = (\beta_2^2/3\beta_3^2 - \beta_1/\beta_3)/3 \quad p = 0, 1, 2, \ldots \end{aligned}\right\} \tag{3.16}$$

For $n = 1$

Taking the b_p to be equal for $p = 1, 2, 3, \ldots$, and the a_p to be equal for $p = 2, 3, 4, \ldots$ reduces the equations to be satisfied to

$$b_p = -\beta_2/3\beta_3 \qquad p = 1, 2, 3, \ldots \qquad (3.17)$$

$$a_p^2 = [\beta_2^2/3\beta_3^2 - \beta_1/\beta_3]/3 \qquad p = 2, 3, 4, \ldots \qquad (3.18)$$

$$a_1^2 + a_0^2 = 2[\beta_2^2/3\beta_3^2 - \beta_1/\beta_3]/3 \qquad (3.19)$$

$$a_1^2 + a_0^2 = 2\beta_2^2/9\beta_3^2 - b_0^2 - 2\beta_2 b_0/3\beta_3 - \beta_1/\beta_3. \qquad (3.20)$$

Equations (3.19) and (3.20) require

$$b_0 = -\beta_2/3\beta_3 \pm [\beta_2^2/9\beta_3^2 - \beta_1/3\beta_3]^{1/2}. \qquad (3.21)$$

Thus if appropriate conditions are satisfied for $n = 0, 1, 2$, the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r \phi_{3r+n}(x) \qquad (3.22)$$

will transform the differential eigenvalue problem

$$\mathscr{L}U + (\beta_3 x^3 + \beta_2 x^2 + \beta_1 x)\rho(x)U = \mu\rho(x)U \qquad (3.23)$$

into an infinite matrix eigenvalue problem of type (2.9).

The results of this Section will be applied to specific orthogonal polynomials, viz. the Jacobi, in Section 4, followed by a discussion of the Fourier functions.

4. The Jacobi polynomials

The Jacobi polynomials $P_p^{\alpha,\beta}(x)$ are solutions of the eigenvalue problem

$$\mathscr{L}U = \frac{d}{dx}\left\{(1-x)^{\alpha+1}(1+x)^{\beta+1}\frac{dU}{dx}\right\} = \lambda(1-x)^{\alpha}(1+x)^{\beta}U \qquad \alpha, \beta > -1 \quad (4.1)$$

in the range $(-1, 1)$ U and $\dfrac{dU}{dx}$ remaining finite at the end points of the range.

The eigenvalues are

$$\lambda_p = -p(p + \alpha + \beta + 1).$$

The recurrence relations satisfied by the normalized polynomials are

$$xP_0^{\alpha,\beta} = a_0 P_1^{\alpha,\beta}(x) + b_0 P_0^{\alpha,\beta}$$

$$xP_p^{\alpha,\beta}(x) = a_p P_{p+1}^{\alpha,\beta}(x) + b_p P_p^{\alpha,\beta}(x) + a_{p-1}P_{p-1}^{\alpha,\beta}(x) \qquad p = 1, 2, 3 \ldots \quad (4.2)$$

where

$$a_0 = \frac{2}{\alpha+\beta+2}\sqrt{\left[\frac{(\alpha+1)(\beta+1)}{\alpha+\beta+3}\right]}, \quad b_0 = \frac{\beta-\alpha}{\alpha+\beta+2}$$

$$a_p = \frac{2}{\alpha+\beta+2p+2} \times \sqrt{\left[\frac{(\alpha+\beta+p+1)(p+1)(\alpha+p+1)(\beta+p+1)}{(\alpha+\beta+2p+1)(\alpha+\beta+2p+3)}\right]}$$

$$b_p = \frac{\beta^2-\alpha^2}{(\alpha+\beta+2p)(\alpha+\beta+2p+2)} \qquad p = 1, 2, 3 \ldots \quad (4.3)$$

The extended eigenvalue problem is

$$\mathscr{L}U + q_2(x)\,\rho(x)\,U = \mu\rho(x)U \qquad (4.4)$$

with the same boundary conditions as those of the operator $\mathscr{L}$. Operators $q_2(x)$ are considered as in Section 3.

(*a*) $q_2(x) = \beta_1 x$

Clearly the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r P_r^{\alpha,\beta}(x) \qquad (4.5)$$

will convert the differential eigenvalue problem (4.4) to the problem of finding the eigenvalues of the infinite tri-diagonal matrix

$$\begin{bmatrix} \beta_1 b_0 & \beta_1 a_0 & & & & \\ \beta_1 a_0 & -(\alpha+\beta+2)+\beta_1 b_1 & \beta_1 a_1 & & & \\ & - & - & - & & \\ & & - & - & & \\ & & & \beta_1 a_{r-1} & -r(r+\alpha+\beta+1)+\beta_1 b_r & \beta_1 a_r \\ & & & & - & - \\ & & & & & - \end{bmatrix} \qquad (4.6)$$

where the a_r and b_r are given by (4.3).

The off-diagonal elements of (4.6) are bounded while the diagonal elements increase in modulus approximately as r^2. The convergence of the eigenvalues obtained from the principal sub-matrices is discussed in Section 6. Inequalities (6.18) and (6.19) give very good indications of the rate of convergence to be expected. The eigenvalues obtained from the principal sub-matrices for certain values of β_1, α and β are given in Tables 7.1 to 7.4.

(*b*) $q_2(x) = \beta_2 x^2 + \beta_1 x$

Condition (3.6)

$$b_p + b_{p+1} = -\beta_1/\beta_2 \qquad p = 0, 1, 2 \ldots$$

is satisfied only if

$$b_p \equiv 0 \qquad p = 0, 1, 2 \ldots$$

i.e.

$$\alpha = \beta \qquad (4.7)$$

$$\beta_1 = 0. \qquad (4.8)$$

Provided (4.7) and (4.8) are satisfied, the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r P_{2r}^{\alpha,\alpha}(x) \tag{4.9}$$

will convert the differential problem (4.4) into the infinite matrix eigenvalue problem shown in (4.10) below

where $a_r = \sqrt{\left[\dfrac{(r+1)(r+2\alpha+1)}{(2r+2\alpha+1)(2r+2\alpha+3)}\right]}$.

The off-diagonal elements are again bounded while the diagonal elements increase in modulus approximately as $4r^2$. The convergence of the eigenvalues of this type of matrix is discussed in Section 6(*b*). Inequalities (6.20) and (6.21) indicate the rate of convergence to be expected. Numerical examples are given in Tables 7.5 and 7.6.

(*c*) $q_2(x) = \beta_3 x^3 + \beta_2 x^2 + \beta_1 x$

Initially expansions involving $n = 0$ and $n = 2$ are considered. To satisfy the b_p conditions of (3.10), (3.12) and (3.14)

$$b_p = \text{constant} = 0 \qquad p = 0, 1, 2, 3, \ldots$$

so that

$$\alpha = \beta \tag{4.11}$$

$$\beta_2 = 0. \tag{4.12}$$

With $n = 0$ conditions (3.11) and the second of (3.12) can be satisfied only if

$$\alpha = -1/2 \tag{4.13}$$

i.e. for the Chebyshev polynomials of the first kind.

In addition β_1 and β_3 must be chosen so that

$$\beta_1 = -3\beta_3/4. \tag{4.14}$$

Thus if (4.11), (4.12), (4.13) and (4.14) hold, the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r P_{3r}^{-1/2,\,-1/2}(x) \tag{4.15}$$

reduces (4.4) to the problem of finding the eigenvalues of the infinite tri-diagonal matrix (4.16) below.

The off-diagonal elements are constant while the diagonal elements increase in modulus as $9r^2$. The matrix is similar to that discussed in Section 6(*a*). The eigenvalues converge very rapidly.

With $n = 2$ the situation is identical with that discussed above except that conditions (3.14) are satisfied by

$$\alpha = 1/2 \tag{4.17}$$

i.e. the Chebyshev polynomials of the second kind.

Thus, subject to conditions (4.11), (4.12), (4.14) and (4.17), the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r P_{3r+2}^{1/2,\,1/2}(x) \tag{4.18}$$

reduces (4.4) to the problem of finding the eigenvalues of the infinite tri-diagonal matrix (4.19) below.

(4.19) is of similar type to (4.16) and the remarks made about the convergence of the eigenvalues of matrix (4.16) apply equally well to those of (4.19).

Returning to the expansion involving $n = 1$, to satisfy the b_p conditions of (3.10) and the first of (3.13)

$$b_p = \text{constant} = 0 \qquad p = 1, 2, 3, \ldots \tag{4.20}$$

$$\begin{bmatrix} \beta_2 a_0^2 & \beta_2 a_0 a_1 & & & & \\ \beta_2 a_0 a_1 & -2(2\alpha+3)+\beta_2(a_2^2+a_1^2) & \beta_2 a_2 a_3 & & & \\ & \text{—} & \text{—} & \text{—} & & \\ & & \text{—} & \text{—} & \text{—} & \\ & & -\beta_2 a_{2r-2} a_{2r-1} & -2r(2r+2\alpha+1)+\beta_2(a_{2r}^2+a_{2r-1}^2) & -\beta_2 a_{2r} a_{2r+1} & \\ & & & \text{—} & \text{—} & \end{bmatrix} \tag{4.10}$$

$$\begin{bmatrix} 0 & \beta_3/4\sqrt{2} & & & & & \\ \beta_3/4\sqrt{2} & -9 & \beta_3/8 & & & & \\ & \text{—} & \text{—} & \text{—} & & & \\ & & & \text{—} & \text{—} & \text{—} & \\ & & & & \beta_3/8 & -9r^2 & \beta_3/8 \\ & & & & & \text{—} & \text{—} & \text{—} \\ & & & & & & \text{—} & \text{—} \end{bmatrix} \tag{4.16}$$

$$\begin{bmatrix} -8 & \beta_3/8 & & & & & \\ \beta_3/8 & -35 & \beta_3/8 & & & & \\ & \text{—} & \text{—} & \text{—} & & & \\ & & & \text{—} & \text{—} & \text{—} & \\ & & & & \beta_3/8 & -(3r+2)(3r+4) & \beta_3/8 \\ & & & & & \text{—} & \text{—} & \text{—} \\ & & & & & & \text{—} & \text{—} \end{bmatrix} \tag{4.19}$$

so that

$$\alpha = \pm\beta \tag{4.21}$$

$$\beta_2 = 0. \tag{4.22}$$

If (4.21) and (4.22) are satisfied, conditions (3.11) and the second of (3.13) can be satified only if either

$$\begin{cases} \alpha = -1/2 \\ \beta = 1/2 \end{cases} \tag{4.23}$$

or

$$\begin{cases} \alpha = 1/2 \\ \beta = -1/2. \end{cases} \tag{4.24}$$

In addition β_1 and β_3 must be chosen so that

$$\beta_1 = -\ 3\beta_3/4. \tag{4.25}$$

The third of conditions (3.13) is also satisfied.

Thus subject to conditions (4.22), (4.25), and either (4.23) or (4.24) the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r P_{3r+1}^{\alpha,\beta}(x) \tag{4.26}$$

reduces (4.4) to the problem of finding the eigenvalues of the infinite tri-diagonal matrix

The third of (4.29) can be written

$$xT_p = (E + E^{-1})T_p/2$$

where E is the displacement operator.

Suppose $q_2(x)$ is a polynomial of degree m, i.e.

$$q_2(x) = \bar{\beta}_2(x^m + \beta_{m-1}x^{m-1} + \ldots + \beta_1 x), \tag{4.30}$$

then

$$q_2(x)T_p = \bar{\beta}_2\left\{\left(\frac{E+E^{-1}}{2}\right)^m + \beta_{m-1}\left(\frac{E+E^{-1}}{2}\right)^{m-1} + \ldots + \beta_1\left(\frac{E+E^{-1}}{2}\right)\right\}T_p. \tag{4.31}$$

For (4.31) to reduce to a 3-term recursion

$$\beta_{m-1} = \beta_{m-3} = \ldots = 0 \tag{4.32}$$

and the non-zero β_i must be the coefficients of powers of $\cos\theta$ in the expansion of $2^{-m+1}\cos m\theta$ viz.

m even

$$\beta_i = \frac{(-1)^{\frac{m+i}{2}} m^2(m^2-2^2)(m^2-4^2)\ldots(m^2-(i-2)^2)}{2^{m-1}(i!)} \tag{4.33}$$

$$\begin{bmatrix} -2 \pm \beta_3/8 & \beta_3/8 & & & & & & \\ \beta_3/8 & -20 & \beta_3/8 & & & & & \\ & — & — & — & & & & \\ & & & & — & — & & \\ & & & & \beta_3/8 & -(3r+1)(3r+2) & \beta_3/8 & \\ & & & & & — & — & — \end{bmatrix} \tag{4.27}$$

(4.23) and (4.24) requiring the positive and negative signs respectively.

This matrix is of similar type to (4.16) and the comments made about the convergence of the eigenvalues of (4.16) apply equally well to those of (4.27).

Thus the only Jacobi polynomials which give infinite symmetrical tri-diagonal matrices when used with a cubic operator $q_2(x)$ are those for which either $\alpha = \beta = \pm 1/2$ or $\alpha = -\beta = \pm 1/2$. The effect of a polynomial operator $q_2(x)$ on these Jacobi polynomials is discussed in the following sub-sections.

(*d*) *Chebyshev polynomials of the first kind $T_p(x)$*

It has been shown that the Chebyshev polynomials of the first kind $T_p(x)$, i.e. the Jacobi polynomials for which

$$\alpha = \beta = -1/2, \tag{4.28}$$

lead to symmetric tri-diagonal matrix eigenvalue problems for certain polynomial operators $q_2(x)$. The effect of a general polynomial operator is now discussed.

The basic recursion of the normalized polynomials is

$$\left.\begin{aligned} xT_0 &= T_1/\sqrt{2} \\ xT_1 &= T_2/2 + T_0/\sqrt{2} \\ xT_p &= (T_{p+1} + T_{p-1})/2 \qquad p = 2, 3, 4, \ldots \end{aligned}\right\} \tag{4.29}$$

m odd

$$\beta_i = \frac{(-1)^{\frac{m+i-2}{2}} m(m^2-1^2)(m^2-3^2)\ldots(m^2-(i-2)^2)}{2^{m-1}(i!)}.$$

With these β_i, (4.31) becomes

$$\begin{aligned} q_2(x)T_p &= \bar{\beta}_2\{2^{-m}(E^m + E^{-m}) + b\}T_p \\ &= \bar{\beta}_2\{2^{-m}T_{p+m} + bT_p + 2^{-m}T_{p-m}\} \end{aligned} \tag{4.34}$$

where $b =$ constant.

(4.34) requires

$$k = m \tag{4.35}$$

and n must be chosen so that the initial 2-term recursion takes the correct form.

The choice of the β_i in (4.32) and (4.33) means that $q_2(x)$ is a multiple of the normalized mth Chebyshev polynomial or differs from one by a constant, i.e.

$$q_2(x) = \bar{\beta}_2 2^{-m}\sqrt{(2\pi)}T_m(x) + \bar{\beta}_1. \tag{4.36}$$

With $n = 0$ the recursions take the required form, viz.

$$\left.\begin{aligned} q_2(x)T_0 &= \bar{\beta}_2 T_m/2^{m-1/2} + \bar{\beta}_1 T_0 \\ q_2(x)T_m &= \bar{\beta}_2 T_{2m}/2^m + \bar{\beta}_1 T_m + \bar{\beta}_2 T_0/2^{m-1/2} \\ q_2(x)T_{mr} &= \bar{\beta}_2\{T_{m(r+1)} + T_{m(r-1)}\}/2^m \\ &\quad + \bar{\beta}_1 T_{mr} \quad r = 2, 3, 4, \ldots \end{aligned}\right\} \tag{4.37}$$

Thus, provided $q_2(x)$ is of form (4.36), the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r T_{mr}(x) \tag{4.38}$$

will reduce

$$\frac{d}{dx}\left(\sqrt{(1-x^2)}\frac{dU}{dx}\right) + \frac{q_2(x)U}{\sqrt{(1-x^2)}} = \frac{\mu U}{\sqrt{(1-x^2)}} \tag{4.39}$$

to the problem of finding the eigenvalues of the infinite tri-diagonal matrix shown in (4.40) below.

Again (4.40) is of similar type to (4.16) and the remarks made about the convergence of the eigenvalues again apply.

(*e*) *Chebyshev polynomials of the second kind* $T_p^*(x)$

These are the Jacobi polynomials for which

$$\alpha = \beta = 1/2 \tag{4.41}$$

and the basic recurrence relations satisfied by the normalized polynomials are

$$\left.\begin{aligned} xT_0^* &= T_1^*/2 \\ xT_p^* &= (T_{p+1}^* + T_{p-1}^*)/2 \qquad p = 1, 2, 3, \ldots \end{aligned}\right\} \tag{4.42}$$

The situation is identical to that described in the previous Section, and for a general polynomial operator $q_2(x)$ of degree m to give the 3-term recursion, conditions (4.32), (4.33) and (4.35) must be satisfied. The desired initial 2-term recursion is obtained if

$$n = m - 1. \tag{4.43}$$

Recursions (4.37) become

$$\left.\begin{aligned} q_2(x)T_{m-1}^* &= \beta_2 T_{2m-1}^*/2^m + cT_{m-1}^* \\ q_2(x)T_{rm+m-1}^* &= \beta_2\{T_{(r+1)m+m-1}^* \\ &\quad + T_{(r-1)m+m-1}^*\}/2^m + cT_{rm+m-1}^* \\ &\qquad r = 1, 2, 3, \ldots \end{aligned}\right\} \tag{4.44}$$

where c is a constant, equal to zero if m is odd. Thus provided $q_2(x)$ satisfies the above conditions the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r T_{(r+1)m-1}(x) \tag{4.45}$$

will reduce

$$\frac{d}{dx}\left\{(1-x^2)^{3/2}\frac{dU}{dx}\right\} + q_2(x)(1-x^2)^{1/2}U = \mu(1-x^2)^{1/2}U \tag{4.46}$$

to the problem of finding the eigenvalues of the infinite tri-diagonal matrix shown in (4.47) below.

Remarks made about the convergence of the eigenvalues of (4.16) also apply to those of the above matrix.

(*f*) *The Jacobi polynomials* $\alpha = -1/2$, $\beta = 1/2$

The basic recurrence relations satisfied by the normalized polynomials are

$$\left.\begin{aligned} xP_0 &= (P_1 + P_0)/2 \\ xP_p &= (P_{p+1} + P_{p-1})/2 \qquad p = 1, 2, 3, \ldots \end{aligned}\right\} \tag{4.48}$$

The situation is again similar to that described in Section 4(*d*). For a general polynomial operator $q_2(x)$ to give the required 3-term recursion, conditions (4.32), (4.33) and (4.35) must be satisfied. The required initial 2-term recursion is then obtained if m is odd and

$$n = (m-1)/2. \tag{4.49}$$

The recursions for $q_2(x)P_p(x)$ then take the form

$$\left.\begin{aligned} q_2(x)P_{(m-1)/2} &= \beta_2(P_{(3m-1)/2} + P_{(m-1)/2})/2^m \\ q_2(x)P_{((2r+1)m-1)/2} &= \beta_2(P_{((2r+3)m-1)/2} \\ &\quad + P_{((2r-1)m-1)/2})/2^m \\ &\qquad r = 1, 2, 3, \ldots \end{aligned}\right\} \tag{4.50}$$

Thus provided $q_2(x)$ satisfies the above conditions the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r P_{((2r+1)m-1)/2}(x) \tag{4.51}$$

$$\begin{bmatrix} \beta_1 & \beta_2/2^{m-1/2} & & & & \\ \beta_2/2^{m-1/2} & -m^2+\beta_1 & \beta_2/2^m & & & \\ & - & - & - & & \\ & & - & - & - & \\ & & & \beta_2/2^m & -m^2r^2+\beta_1 & \beta_2/2^m \\ & & & & - & - & - \\ & & & & & - & - \end{bmatrix} \tag{4.40}$$

$$\begin{bmatrix} -(m^2-1)+c & \beta_2 2^{-m} & & & & \\ \beta_2 2^{-m} & -(4m^2-1)+c & \beta_2 2^{-m} & & & \\ & - & - & - & & \\ & & - & - & - & \\ & & & \beta_2 2^{-m} & -\{(r+1)^2m^2-1\}+c & \beta_2 2^{-m} \\ & & & & - & - \end{bmatrix} \tag{4.47}$$

will reduce

$$\frac{d}{dx}\left\{(1-x)^{1/2}(1+x)^{3/2}\frac{dU}{dx}\right\} + q_2(x)\left(\frac{1+x}{1-x}\right)^{1/2}U = \mu\left(\frac{1+x}{1-x}\right)^{1/2}U \quad (4.52)$$

to the problem of finding the eigenvalues of the infinite tri-diagonal matrix

$$\begin{bmatrix} \beta_2 2^{-m} - (m^2-1)/4 & \beta_2 2^{-m} & & & & \\ \beta_2 2^{-m} & -(9m^2-1)/4 & \beta_2 2^{-m} & & & \\ & - & - & - & & \\ & & - & - & - & \\ & & & \beta_2 2^{-m} & -((2r+1)^2m^2-1)/4 & \beta_2 2^{-m} \\ & & & & - & - \end{bmatrix} \quad (4.53)$$

Comments made about the convergence of the eigenvalues of (4.16) also apply to those of the above matrix.

(*g*) *Jacobi polynomials* $\alpha = 1/2$, $\beta = -1/2$

The analysis follows an identical pattern to that described in the previous sub-section, but the first of recursions (4.48) and (4.50) are replaced, respectively, by

$$xP_0 = (P_1 - P_0)/2 \quad (4.54)$$

$$q_2(x)P_{(m-1)/2} = \beta_2(P_{(3m-1)/2} - P_{(m-1)/2})/2^m \quad (4.55)$$

and equation (4.52) by

$$\frac{d}{dx}\left\{(1+x)^{1/2}(1-x)^{3/2}\frac{dU}{dx}\right\} + q_2(x)\left(\frac{1-x}{1+x}\right)^{1/2}U = \mu\left(\frac{1-x}{1+x}\right)^{1/2}U. \quad (4.56)$$

The resulting infinite tri-diagonal matrix has the same elements as (4.53) except that the first becomes $-\beta_2 2^{-m} - (m^2-1)/4$.

5. Fourier functions

The next orthogonal functions discussed are the Fourier Sine and Cosine functions which are very closely related to the Chebyshev polynomials, and the conclusions are equivalent.

(*a*) *Sine functions*

The Fourier Sine functions

$$\phi_p(x) = \sqrt{(2/\pi)}\sin px \qquad p = 1, 2, 3, \ldots \quad (5.1)$$

are an orthonormal set in the range $(0, \pi)$ being solutions of the eigenvalue problem

$$\mathscr{L}U = \frac{d^2U}{dx^2} = \lambda U \quad (5.2)$$

with the boundary conditions which may take the form

$$\left.\begin{aligned} U(0) &= 0 \\ U(\pi) &= 0 \end{aligned}\right\} \quad (5.3)$$

and with eigenvalues

$$\lambda_p = -p^2 \qquad p = 1, 2, 3, \ldots \quad (5.4)$$

The recurrence relations satisfied by the $\phi_p(x)$ are

$$\left.\begin{aligned} (\cos x)\phi_1 &= \phi_2/2 \\ (\cos x)\phi_p &= (\phi_{p+1} + \phi_{p-1})/2 \qquad p = 2, 3, 4, \ldots \end{aligned}\right\} \quad (5.5)$$

The extended eigenvalue problem is

$$\mathscr{L}U + q_2(x)U = \mu U \quad (5.6)$$

with any boundary conditions for which the $\phi_p(x)$ satisfy (1.2).

(*i*) $q_2(x) = \beta_1 \cos x$

This is the Mathieu problem discussed in this connection by Mayers (Fox, 1961).

Clearly the recursions are of the form (2.8) with $k = 1$, $n = 1$, and the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r \phi_{r+1}(x) \quad (5.7)$$

will reduce (5.6) to the problem of finding the eigenvalues of the infinite tri-diagonal matrix

$$\begin{bmatrix} -1^2 & \beta_1/2 & & & & \\ \beta_1/2 & -2^2 & \beta_1/2 & & & \\ & - & - & - & & \\ & & - & - & - & \\ & & & \beta_1/2 & -r^2 & \beta_1/2 \\ & & & & - & - & - \\ & & & & & - & - & - \end{bmatrix} \quad (5.8)$$

The convergence of the eigenvalues obtained from the principal sub-matrices of (5.8) is discussed in Section 6(*a*) where expressions (6.13) and (6.14) give very good estimates of the rate of convergence to be expected. Numerical examples are given in Tables 7.7. and 7.8.

(ii) $q_2(x)$ = *polynomial of degree m in cos x*

The situation is identical to that discussed in Section 4(*e*), i.e. the Chebyshev polynomials of the second kind. In order that $q_2(x)\phi_p(x)$ should give the required recursion, the operator $q_2(x)$ must either be a multiple $\cos mx$ or differ from one by a constant, i.e.

$$q_2(x) = \beta_2 \cos mx + \beta_1 \tag{5.9}$$

so that

$$\left.\begin{aligned} q_2(x)\phi_m &= \beta_2\phi_{2m}/2 + \beta_1\phi_m \\ q_2(x)\phi_{mr} &= \beta_2\{\phi_{m(r+1)} + \phi_{m(r-1)}\}/2 + \beta_1\phi_{mr} \\ &\qquad r = 2, 3, 4, \ldots \end{aligned}\right\} \tag{5.10}$$

The substitution

$$U = \sum_{r=0}^{\infty} \alpha_r \phi_{mr+m}(x) \tag{5.11}$$

will then reduce (5.6) to the problem of finding the eigenvalues of the infinite tri-diagonal matrix (5.12) below.

The eigenvalues obtained from the principal sub-matrices of (5.12) will converge in an identical manner to those of (5.8).

(*b*) *Cosine functions*

The Fourier Cosine functions

$$\left.\begin{aligned} \phi_0 &= 1/\sqrt{\pi} \\ \phi_p(x) &= \sqrt{(2/\pi)}\cos px \quad p = 1, 2, 3, \ldots \end{aligned}\right\} \tag{5.13}$$

are an orthonormal set in the range $(0, \pi)$ being solutions of the eigenvalue problem

$$\mathscr{L}U = \frac{d^2U}{dx^2} = \lambda U \tag{5.14}$$

with boundary conditions which may take the form

$$\left.\begin{aligned} U'(0) &= 0 \\ U'(\pi) &= 0 \end{aligned}\right\} \tag{5.15}$$

and with eigenvalues

$$\lambda_p = -p^2 \quad p = 0, 1, 2, \ldots. \tag{5.16}$$

The recurrence relations satisfied by the $\phi_p(x)$ are

$$\left.\begin{aligned} (\cos x)\phi_0 &= \phi_1/\sqrt{2} \\ (\cos x)\phi_1 &= \phi_2/2 + \phi_0/\sqrt{2} \\ (\cos x)\phi_p &= (\phi_{p+1} + \phi_{p-1})/2 \quad p = 2, 3, 4, \ldots. \end{aligned}\right\} \tag{5.17}$$

The extended eigenvalue problem is

$$\mathscr{L}U + q_2(x)U = \mu U \tag{5.18}$$

with appropriate boundary conditions.

(i) $q_2(x) = \beta_1 \cos x$

Clearly the recursion obtained by operating $q_2(x)$ on $\phi_p(x)$ is of the form (2.8) with $k = 1$, $n = 0$, and the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r \phi_r(x) \tag{5.19}$$

will reduce (5.18) to the problem of finding the eigenvalues of the infinite tri-diagonal matrix (5.20) below.

The comments made about the convergence of the eigenvalues of (5.8) apply equally well to those of (5.20). Numerical examples are given in Tables 7.9 and 7.10.

(ii) $q_2(x)$ = *polynomial of degree m in cos x*

As in Section 5(*a*) (ii), in order to obtain the appropriate recurrence relations when $q_2(x)$ operates on $\phi_p(x)$, $q_2(x)$ must reduce to form (5.9). The recursions then take the form

$$\left.\begin{aligned} q_2(x)\phi_0 &= \beta_2\phi_m/\sqrt{2} + \beta_1\phi_0 \\ q_2(x)\phi_m &= \beta_2(\phi_{2m}/2 + \phi_0/\sqrt{2}) + \beta_1\phi_m \\ q_2(x)\phi_{mr} &= \beta_2(\phi_{m(r+1)} + \phi_{m(r-1)})/2 + \beta_1\phi_{mr} \\ &\qquad r = 2, 3, \ldots \end{aligned}\right\} \tag{5.21}$$

$$\begin{bmatrix} \beta_1 - m^2 & \beta_2/2 & & & & & & & \\ \beta_2/2 & \beta_1 - 4m^2 & \beta_2/2 & & & & & & \\ & \text{—} & \text{—} & \text{—} & & & & & \\ & & & \text{—} & \text{—} & \text{—} & & & \\ & & & & \beta_2/2 & \beta_1 - r^2m^2 & \beta_2/2 & & \\ & & & & & \text{—} & \text{—} & \text{—} & \\ & & & & & & \text{—} & \text{—} & \text{—} \end{bmatrix} \tag{5.12}$$

$$\begin{bmatrix} 0 & \beta_1/\sqrt{2} & & & & & & & \\ \beta_1/\sqrt{2} & -1^2 & \beta_1/2 & & & & & & \\ & \beta_1/2 & -2^2 & \beta_1/2 & & & & & \\ & & \text{—} & \text{—} & \text{—} & & & & \\ & & & & \text{—} & \text{—} & \text{—} & & \\ & & & & & \beta_1/2 & -r^2 & \beta_1/2 & \\ & & & & & & \text{—} & \text{—} & \text{—} \\ & & & & & & & \text{—} & \text{—} \end{bmatrix} \tag{5.20}$$

and the substitution

$$U = \sum_{r=0}^{\infty} \alpha_r \phi_{mr}(x) \tag{5.22}$$

will reduce (5.18) to the problem of finding the eigenvalues of the infinite tri-diagonal matrix (5.23) below.

Again the comments made about the convergence of the eigenvalues of (5.8) apply to (5.23).

6. Convergence of the eigenvalues

(*a*) First consider the infinite symmetric tri-diagonal matrix (6.1) below, where q is a constant.

Bounds are now obtained for the difference between the eigenvalues of the matrix of the first n rows and columns of (6.1), and those of the matrix of the first $(n+1)$ rows and columns.

Consider the matrix S_n (see (6.2) below).

Let μ_n be an eigenvalue of S_n and $\boldsymbol{x}$ the corresponding eigenvector normalized to have Euclidean length unity, i.e.

$$S_n \boldsymbol{x} = \mu_n \boldsymbol{x} \tag{6.3}$$

$$\boldsymbol{x}^T \boldsymbol{x} = 1. \tag{6.4}$$

Then

$$\left.\begin{aligned} S_{n+1}\begin{bmatrix} \boldsymbol{x} \\ 0 \end{bmatrix} &= \begin{bmatrix} S_n & q\boldsymbol{e}_n \\ q\boldsymbol{e}_n^T & -(n+1)^2 \end{bmatrix}\begin{bmatrix} \boldsymbol{x} \\ 0 \end{bmatrix} \\ &= \begin{bmatrix} S_n \boldsymbol{x} \\ q\boldsymbol{e}_n^T \boldsymbol{x} \end{bmatrix} \\ &= \mu_n \begin{bmatrix} \boldsymbol{x} \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ q\alpha_n \end{bmatrix} \end{aligned}\right\} \tag{6.5}$$

where $\boldsymbol{e}_n$ is the last column of the unit matrix of order n and α_n is the last element of $\boldsymbol{x}$.

Wilkinson's application of Rayleigh's Theorem (Wilkinson, 1961) shows that at least one eigenvalue μ_{n+1} lies in the interval

$$|\mu_n - \mu_{n+1}| \leqslant |q\alpha_n|. \tag{6.6}$$

If the Gershgorin circles of S_n (Gershgorin, 1937) are examined, it is clear that they are centred at $-1, -4, \ldots, -s^2, \ldots, -n^2$, and have the same radius $2|q|$ except the first and the last which both have radius $|q|$. Clearly if n is large enough, a positive integer r can be found such that all circles centred to the right of $-r^2$ overlap, while the one centred at $-r^2$ and those to the left are disjoint. In fact r is the least integer such that

$$2r - 1 > 4|q|. \tag{6.7}$$

$$\begin{bmatrix} \beta_1 & \beta_2/\sqrt{2} & & & & & \\ \beta_2/\sqrt{2} & -m^2+\beta_1 & \beta_2/2 & & & & \\ & \beta_2/2 & -m^2 2^2+\beta_1 & \beta_2/2 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \beta_2/2 & -m^2 r^2 + \beta_1 & \beta_2/2 & \\ & & & & \ddots & \ddots & \ddots \end{bmatrix} \tag{5.23}$$

$$\begin{bmatrix} -1 & q & & & & \\ q & -4 & q & & & \\ & \ddots & \ddots & \ddots & & \\ & & q & -s^2 & q & \\ & & & \ddots & \ddots & \ddots \end{bmatrix} \tag{6.1}$$

$$S_n = \begin{bmatrix} -1 & q & & & & \\ q & -4 & q & & & \\ & \ddots & \ddots & \ddots & & \\ & & q & -s^2 & q & \\ & & & \ddots & \ddots & \ddots \\ & & & & q & -n^2 \end{bmatrix} \tag{6.2}$$

If $\mu_n^{(i)}$ is the ith eigenvalue of S_n arranged in order of descending algebraic value,

$$\mu_n^{(i)} > -(r-1)^2 - 2|q| > -r^2 + 2|q| \qquad (6.8)$$

$$i = r-1, r-2, \ldots, 1$$

$$\mu_n^{(i)} > -i^2 - 2|q| > -(i+1)^2 + 2|q| \qquad (6.9)$$

$$i = r, r+1, \ldots, n.$$

Now consider the equations satisfied by certain of the elements of x

$$\left.\begin{array}{ll} q\alpha_{s-1} - (\mu_n^{(i)} + s^2)\alpha_s + q\alpha_{s+1} & = 0 \\ q\alpha_s - (\mu_n^{(i)} + (s+1)^2)\alpha_{s+1} + q\alpha_{s+2} & = 0 \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots & \\ q\alpha_{n-1} - (\mu_n^{(i)} + n^2)\alpha_n & = 0 \end{array}\right\} \qquad (6.10)$$

First assume $q > 0$ and $i < r$, and choose $\alpha_n > 0$, then using (6.8)

$$\alpha_n < \alpha_{n-1} < \alpha_{n-2} \ldots < \alpha_{r-1} \leqslant 1 \qquad (6.11)$$

and

$$\alpha_n < \frac{q}{\mu_n^{(i)} + n^2}\,\frac{q}{\mu_n^{(i)} + (n-1)^2 - q}\cdots\frac{q\alpha_{r-1}}{\mu_n^{(i)} + r^2 - q}$$

$$< \frac{q}{n^2 - r^2}\cdot\frac{q}{(n-1)^2 - r^2}\cdots\frac{q}{(r+1)^2 - r^2}\cdot\frac{q}{q} \qquad (6.12)$$

$$\therefore \qquad \alpha_n < \frac{q^{n-r}(2r)!}{(n+r)!(n-r)!}.$$

Substituting in (6.6) gives

$$|\mu_n^{(i)} - \mu_{n+1}^{(i)}| < \frac{q^{n-r+1}(2r)!}{(n+r)!(n-r)!} \qquad (6.13)$$

$$i = r-1, r-2, \ldots, 1.$$

Similarly

$$|\mu_n^{(i)} - \mu_{n+1}^{(i)}| < \frac{q^{n-i}(2i+2)!}{(n+i+1)!(n-i-1)!} \qquad (6.14)$$

$$i = r, r+1, \ldots, n-1.$$

For $q < 0$ the same argument gives identical expressions except that q is replaced by $|q|$.

It should be noted that inequalities (6.13) and (6.14) hold for the eigenvalues μ_{n+m} of matrix S_{n+m} since

$$S_{n+m}\begin{bmatrix} x \\ 0 \end{bmatrix} = \begin{bmatrix} S_n x \\ q\alpha_n \\ 0 \end{bmatrix} = \mu_n\begin{bmatrix} x \\ \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ q\alpha_n \\ 0 \end{bmatrix}.$$

The sequences of corresponding eigenvalues obtained from the matrices $S_n, S_{n+1}, \ldots$ satisfy Cauchy's principle of convergence, i.e. corresponding to any given positive number ϵ there exists an n such that

$$|\mu_n^{(i)} - \mu_{n+m}^{(i)}| < \epsilon$$

for all positive integral m. Thus the eigenvalues converge and the limit lies in the range

$$\mu_n^{(i)} \pm |q\alpha_n|.$$

Inequalities (6.13) and (6.14) give very good guides to the order of matrix to be used to obtain a specified accuracy.

However, when the eigenvalues and eigenvectors of S_n have been calculated, better bounds than those given by (6.13) and (6.14) can be obtained. Now $\mu_n^{(i)}$ is the Rayleigh quotient for vector $\begin{bmatrix} x \\ 0 \end{bmatrix}$ and matrix S_{n+1}. Assuming that there is only one eigenvalue $\mu_{n+1}^{(i)}$ of S_{n+1} which satisfies (6.6) while all others satisfy

$$|\mu_n^{(i)} - \mu_{n+1}^{(j)}| \geqslant a \qquad j \neq i, \qquad (6.15)$$

then the application of Wilkinson's "improved" bound (Wilkinson, 1961) gives the inequality

$$|\mu_n^{(i)} - \mu_{n+1}^{(i)}| \leqslant \frac{q^2\alpha_n^2}{a\left(1 - \dfrac{q^2\alpha_n^2}{a^2}\right)}. \qquad (6.16)$$

Numerical examples of the eigenvalues of matrix (6.2) are given in Tables 7.7. and 7.8 with $q = \beta_1/2$.

(b) Jacobi polynomials

If the above technique is applied to matrix (4.6), the following inequalities are obtained.

$$|\mu_n^{(i)} - \mu_{n+1}^{(i)}| < \frac{|\beta_1|^{n-r+1}a_n a_{n-1}\ldots a_r}{\{n(n+\alpha+\beta+1) - r(r+\alpha+\beta+1)\}\{(n-1)(n+\alpha+\beta) - r(r+\alpha+\beta+1)\}\ldots\{(r+1)(r+\alpha+\beta+2) - r(r+\alpha+\beta+1)\}}$$

$$i = r-1, r-2, \ldots, 0, \qquad (6.18)$$

$$|\mu_n^{(i)} - \mu_{n+1}^{(i)}| < \frac{|\beta_1|^{n-i}a_n a_{n-1}\ldots a_{i+1}}{\{n(n+\alpha+\beta+1) - (i+1)(i+2+\alpha+\beta)\}\ldots\{(i+2)(i+3+\alpha+\beta) - (i+1)(i+\alpha+\beta+2)\}}$$

$$i = r, r+1, r+2, \ldots, n-1, \qquad (6.19)$$

where r is the smallest positive integer such that

$$2r + \alpha + \beta - \beta_1(b_r - b_{r-1}) > |\beta_1|(a_r + 2a_{r-1} + a_{r-2}).$$

Clearly the eigenvalues obtained by repeated bordering of the principal sub-matrix of (4.6) will converge very rapidly, and (6.18) and (6.19) give good estimates of the order of matrix required to give a specified accuracy. Numerical examples are given in Tables 7.1 to 7.4. A numerical comparison of inequality (6.18) and the equivalent of (6.16) for one of the eigenvalues of Table 7.4 is given in Table 7.12.

The corresponding inequalities for matrix (4.10) are

$$|\mu_n^{(i)} - \mu_{n+1}^{(i)}| <$$

$$\frac{|\beta_2|^{n-r+1}a_{2n}a_{2n+1}a_{2n-2}a_{2n-1}\ldots a_{2r}a_{2r+1}}{\{2n(2n+2\alpha+1) - 2(i+1)(2i+2\alpha+3)\}\ldots\{2(r+1)(2r+2\alpha+3) - 2r(2r+2\alpha+1)\}}$$

$$i = r-1, r-2, \ldots, 0. \qquad (6.20)$$

$$|\mu_n^{(i)} - \mu_{n+1}^{(i)}| <$$

$$\frac{|\beta_2|^{n-i}a_{2n}a_{2n+1}\ldots a_{2i+2}a_{2i+3}}{\{2n(2n+2\alpha+1) - 2(i+1)(2i+2\alpha+3)\}\ldots\{2(i+2)(2i+2\alpha+5) - 2(i+1)(2i+2\alpha+3)\}}$$

$$i = r, r+1, \ldots, n-1. \qquad (6.21)$$

where r is the least positive integer such that

$$2(4r + 2\alpha - 1) + \beta_2(a_{2r-2}^2 + a_{2r-3}^2 - a_{2r}^2 - a_{2r-1}^2) > |\beta_2|(a_{2r}a_{2r+1} + 2a_{2r-2}a_{2r-1} + a_{2r-4}a_{2r-3}). \qquad (6.22)$$

Again the eigenvalues obtained by repeated bordering of the principal sub-matrix will converge very rapidly. Numerical examples are given in Tables 7.5 and 7.6.

7. Numerical examples

The following tables give the eigenvalues of some of the matrices discussed in the previous Sections, n being the order of the matrix. The eigenvalues of the lowest order matrix, and the additional eigenvalues obtained after each bordering are given in full, but only the significant digits that have changed are given subsequently. The row marked "R" contains the most significant digits that have been repeated.

It should be noted that when constants β_i appear only in the off-diagonal elements, the eigenvalues are unaltered if β_i is replaced by $-\beta_i$, so that negative values of β_i were not considered in these cases.

The eigenvalues were obtained by the method of bisections described, for example, in *Modern Computing Methods* and are given to an accuracy

$$x_0 \leqslant \mu \leqslant x_1$$

where

$$|x_1 - x_0| \leqslant 10^{-7}|\mu| + 10^{-17}.$$

The eigenvectors were also calculated, normalized so that the largest element is unity, but space prevents their inclusion in full in the paper. However, Table 7.11 gives a typical example, the elements being given in floating-point form.

The calculations were made using the University of London's Mercury computer.

A comparison of the theoretical rate of convergence and the actual rate for one of the eigenvalues of Table 7.4 is given in Table 7.12.

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(*Tables overleaf*)

Table 7.1

Jacobi polynomials (1/2, −1/2) Matrix (4.6) α = 1/2 β = −1/2

$\beta_1 = -3$

n	$\mu^{(0)}$	$\mu^{(1)}$	$\mu^{(2)}$	$\mu^{(3)}$	$\mu^{(4)}$	$\mu^{(5)}$	$\mu^{(6)}$
4	2·090978	−2·034822	−6·19004	−12·36612			
5		478	8092	09843	−20·27716		
6		7	85	426	05859	−30·22280	
7				4	636	03886	−42·18619
8						753	02765
9							680
R	2·090978	−2·034477	−6·18085	−12·09424	−20·05636	−30·03753	−42·02

Table 7.2

$\beta_1 = 3$

n	$\mu^{(0)}$	$\mu^{(1)}$	$\mu^{(2)}$	$\mu^{(3)}$	$\mu^{(4)}$	$\mu^{(5)}$	$\mu^{(6)}$
4	−0·053627	−2·866793	−6·21341	−12·36617			
5	570	402	0438	09849	−20·27716		
6		0	2	432	05859	−30·22280	
7				0	636	03886	−42·18619
8						753	02765
9							680
R	−0·053570	−2·866400	−6·20432	−12·09430	−20·05636	−30·03753	−42·02

Table 7.3

Legendre polynomials (*a*) Matrix (4.6) α = β = 0

$\beta_1 = 3$

n	$\mu^{(0)}$	$\mu^{(1)}$	$\mu^{(2)}$	$\mu^{(3)}$	$\mu^{(4)}$	$\mu^{(5)}$	$\mu^{(6)}$
4	1·092649	−2·478415	−6·23732	−12·37691			
5	70	7976	2785	10528	−20·28156		
6		4	78	101	06086	−30·22505	
7				099	5860	03984	−42·18749
8					59	850	02814
9							729
R	1·092670	−2·477974	−6·22778	−12·10099	−20·05859	−30·03850	−42·02

Table 7.4

$\beta_1 = 7$

n	$\mu^{(0)}$	$\mu^{(1)}$	$\mu^{(2)}$	$\mu^{(3)}$	$\mu^{(4)}$	$\mu^{(5)}$	$\mu^{(6)}$
4	3·778196	−2·503256	−7·38575	−13·88919			
5	80119	459438	19126	−12·68135	−21·44808		
6	51	8198	8190	58076	−20·38204	−31·17726	
7		83	74	7812	2390	−30·24687	−42·99134
8				10	292	1099	17263
9						56	4908
R	3·780151	−2·458183	−7·18174	−12·57810	−20·32292	−30·210	−42·1

Table 7.5

Legendre polynomials (*b*) Matrix (4.10) $\alpha = \beta = 0$

$\beta_2 = -3$

n	$\mu^{(0)}$	$\mu^{(1)}$	$\mu^{(2)}$	$\mu^{(3)}$	$\mu^{(4)}$	$\mu^{(5)}$	$\mu^{(6)}$
4	−0·879934	−7·64932	−21·53565	−43·53510			
5			4	1619	−73·5242		
6				9	093	−111·5183	
7						060	−157·5147
8							042
R	−0·879934	−7·64932	−21·53564	−43·51619	−73·5093	−111·5060	−157·5

Table 7.6

$\beta_2 = 3$

n	$\mu^{(0)}$	$\mu^{(1)}$	$\mu^{(2)}$	$\mu^{(3)}$	$\mu^{(4)}$	$\mu^{(5)}$	$\mu^{(6)}$
4	1·144328	−4·531027	−18·49641	−40·51689			
5			40	49799	−70·5136		
6					4988	−108·5115	
7						4992	−154·5099
8							4994
R	1·144328	−4·531027	−18·49640	−40·49799	−70·4988	−108·4992	−154

Table 7.7

Fourier sine functions Matrices (5.8) and (6.2)

$\beta_1 = 6$ ($q = 3$)

n	$\mu^{(0)}$	$\mu^{(1)}$	$\mu^{(2)}$	$\mu^{(3)}$	$\mu^{(4)}$	$\mu^{(5)}$	$\mu^{(6)}$
5	1·140882	−4·348921	−9·50340	−16·33234	−25·95622		
6	5	813	152	28980	20801	−36·77928	
7		2	0	17	18297	14213	−49·67631
8					71	2628	10309
9						16	09248
10							2
R	1·140885	−4·348812	−9·50150	−16·28917	−25·18271	−36·12616	−49·0924

Table 7.8

$\beta_1 = 14$ ($q = 7$)

n	$\mu^{(0)}$	$\mu^{(1)}$	$\mu^{(2)}$	$\mu^{(3)}$	$\mu^{(4)}$	$\mu^{(5)}$	$\mu^{(6)}$
5	6·38954	−2·807643	−10·74138	−18·32756	−29·51295		
6	9041	781119	56691	−17·63852	−26·53430	−39·86956	
7	3	0173	5648	56983	04915	−37·05434	−52·3805
8		56	21	721	1770	−36·71019	−49·76244
9				17	690	69448	51452
10					89	18	0608
R	6·39043	−2·780156	−10·55621	−17·56717	−26·016	−36·694	−49·5

Table 7.9

Fourier cosine functions Matrix 5.20

$\beta_1 = 6$

n	$\mu^{(0)}$	$\mu^{(1)}$	$\mu^{(2)}$	$\mu^{(3)}$	$\mu^{(4)}$	$\mu^{(5)}$	$\mu^{(6)}$
5	4·332990	−1·721606	−5·75158	−9·65789	−17·20191		
6	3016	19707	4317	58112	−16·33280	−25·95622	
7	7	684	03	7928	29027	20801	−36·79274
8				6	8964	18297	14212
9						72	2628
10						1	16
R	4·333017	−1·719684	−5·74303	−9·57926	−16·28964	−25·1827	−36·126

Table 7.10

$\beta_1 = 14$

n	$\mu^{(0)}$	$\mu^{(1)}$	$\mu^{(2)}$	$\mu^{(3)}$	$\mu^{(4)}$	$\mu^{(5)}$	$\mu^{(6)}$
5	11·41641	1·533415	−7·56130	−13·95481	−21·43372		
6	828	640672	−6·90054	−13·12422	−18·52045	−29·51375	
7	34	6841	82441	−12·95067	−17·88346	−26·53708	−39·86957
8		7013	090	3790	1929	−26·05245	−37·05435
9		6	83	53	681	2103	−36·71021
10				2	77	023	69449
R	11·41834	1·647016	−6·82083	−12·9375	−17·816	−26·02	−36

Table 7.11

Eigenvectors of the eigenvalue $\mu^{(0)}$ of Table 7.4

$n = 4$	$n = 5$	$n = 6$	$n = 7$	$n = 8$	$n = 9$
1·000000 0	1·000000 0	1·000000 0	1·000000 0	1·000000 0	1·000000 0
9·348611 −1	9·353370 −1	9·353447 −1	9·353448 −1	9·353448 −1	9·353448 −1
3·763321 −1	3·775903 −1	3·776108 −1	3·776109 −1	3·776109 −1	3·776109 −1
8·466407 −2	8·758015 −2	8·790189 −2	8·790231 −2	8·790231 −2	8·790231 −2
	1·303215 −2	1·324382 −2	1·324555 −2	1·324555 −2	1·324555 −2
		1·379120 −3	1·390391 −3	1·390442 −3	1·390442 −3
			1·066697 −4	1·071557 −4	1·071570 −4
				6·289803 −6	6·307003 −6
					2·918673 −7

Table 7.12

Comparison of theoretical and actual rates of convergence for $\mu^{(0)}$ of Table 7.4

n	$\mu^{(0)}$	α_n	a	$\epsilon = \left\lvert \frac{7n}{\sqrt{(4n^2 - 1)}} \alpha_n \right\rvert$	$\frac{\epsilon^2}{a(1 - \epsilon^2/a^2)}$	$\mu_{n+1}^{(0)} - \mu_n^{(n)}$
4	3·778196	8·4664 −2	$\simeq 6$	2·9866 −1	1·4903 −2	0·001923
5	3·780119	1·3032 −2	$\simeq 6$	4·5842 −2	3·5025 −4	0·000030
6	3·780151	1·3791 −3	$\simeq 6$	4·8438 −3	3·9104 −6	0·000000