The numerical solution of eigenvalue problems in which the eigenvalue parameter appears nonlinearly, with an application to differential equations

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Formulae are constructed which permit the efficient numerical solution of eigenvalue problems in which the eigenvalue parameter appears nonlinearly. Problems of this type can occur in the numerical solution by finite-difference methods of the eigenvalue problems of ordinary differential equations.

1. Introduction

In a recent paper (Osborne, 1962) we discuss finite-difference methods for solving the eigenvalue problems of ordinary differential equations. In particular (in Sections 3 and 5 of that paper) an approximate eigenvalue of the finite-difference equations is refined by methods which are essentially Newton's method applied to certain implicitly defined functions of the eigenvalue. This work is continued in this paper where (in Section 3) we use similar techniques to derive iterative formulae for refining approximate solutions to eigenvalue problems in which the eigenvalue parameter appears nonlinearly. This work is motivated in Section 2 where we discuss examples of finite-difference approximations to differential equation eigenvalue problems. We exemplify some of our formulae in Section 4.

In Section 3 we write $\frac{dV}{d\lambda}$ for the vector whose components are obtained by differentiating the corresponding components of V with respect to λ. The pth component of $\frac{dV}{d\lambda}$ is written $\left(\frac{dV}{d\lambda}\right)_p$.

2. Some finite-difference approximations

In this Section we derive finite-difference formulae for approximating to the eigenvalue problems of ordinary differential equations. These formulae have the characteristic feature that the eigenvalue parameter appears nonlinearly in them. The cases we consider are (*a*) approximation by standard methods to the differential equation at a singular point caused either by a singular coefficient or by a boundary point at ∞, and (*b*) approximation by a somewhat non-standard method at a regular point.

We consider first Legendre's equation

$$\frac{d}{dx}\left[(1-x^2)\frac{dP}{dx}\right]+\lambda P=0. \tag{2.1}$$

We seek those solutions which are regular at $x=\pm 1$. Writing the equation in the form

$$\frac{d^2P}{dx^2}+\frac{1}{1-x^2}\left(-2x\frac{dP}{dx}+\lambda P\right)=0, \tag{2.2}$$

we see that necessarily these solutions satisfy

$$2\frac{dP}{dx}+\lambda P=0,\ x=-1,$$

$$-2\frac{dP}{dx}+\lambda P=0,\ x=+1. \tag{2.3}$$

Also, by letting x tend to $+1$, -1 in equation (2.2) and using equation (2.3) we find that the regular solutions satisfy

$$2\frac{d^2P}{dx^2}-\left(1-\frac{\lambda}{2}\right)\frac{dP}{dx}=0,\ x=-1,$$

$$2\frac{d^2P}{dx^2}+\left(1-\frac{\lambda}{2}\right)\frac{dP}{dx}=0,\ x=+1. \tag{2.4}$$

Equations (2.3) and (2.4) can be approximated by the usual finite-difference techniques. For example, if we make the usual central-difference approximations to the equations holding at $x=-1$, and then eliminate $P(-1-h)$ between them, we find the relation

$$\left[-1+\frac{\lambda h}{8}(4+h)-\frac{\lambda^2h^2}{16}\right]P(-1)+P(-1+h)=0 \tag{2.5}$$

where h is the mesh spacing. We note that equation (2.5) depends nonlinearly on λ.

A problem of a different kind occurs when one boundary point is at ∞. Consider the example

$$\frac{d^2P}{dx^2}+(\lambda+q(x))P=0, \tag{2.6}$$

where $\int_0^\infty |q(x)|dx<\infty$, subject to the boundary conditions

$$P(0)=0,\ \int_0^\infty P^2dx<\infty. \tag{2.7}$$

The differential equation is of limit-point type at ∞ so that at most one solution can satisfy the second of the conditions (2.7) for any value of $\lambda<0$, while it can be satisfied by no solution for $\lambda>0$. We attempt to incorporate this condition into our working by matching to

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an appropriate asymptotic solution to (2.6) for some sufficiently large value of x. For example, if the W.K.B. method adequately represents the solutions of (2.6) then the appropriate solution is

$$y = \frac{1}{[4|\lambda + q(x)|]^{1/4}} e^{-\eta(x)} \tag{2.8}$$

where $\eta(x) = \int^x |\lambda + q(t)|^{1/2} dt$.

To match on to the asymptotic form at $x = x_n = nh$ we use the difference relation

$$P(x_{n-1}) - P(x_n)\frac{y(x_{n-1})}{y(x_n)} = 0. \tag{2.9}$$

Substituting from equation (2.8) gives

$$P(x_{n-1}) - \left|\frac{\lambda + q(x_n)}{\lambda + q(x_{n-1})}\right|^{1/4} \exp\left\{\frac{h}{2}(|\lambda + q(x_n)|^{1/2} + |\lambda + q(x_{n-1})|^{1/2})\right\} P(x_n) = 0, \tag{2.10}$$

where we have used the trapezoidal rule to estimate the integral of η. Again λ enters nonlinearly in equation (2.10).

The difference approximation at a regular point which is to be our second example follows readily from the observation that any solution to an ordinary linear differential equation also satisfies exactly a difference equation of the same order. To show this we consider the differential equation

$$\frac{d^2P}{dx^2} + q(x, \lambda)P = 0. \tag{2.11}$$

We assume that we know a fundamental set of solutions $V(x)$ and $U(x)$. Then if the difference equation is

$$A_{i-1}P(x_{i-1}) + A_iP(x_i) + A_{i+1}P(x_{i+1}) = 0, \tag{2.12}$$

we must have

$$A_{i-1}V(x_{i-1}) + A_iV(x_i) + A_{i+1}V(x_{i+1}) = 0,$$
$$\text{and} \quad A_{i-1}U(x_{i-1}) + A_iU(x_i) + A_{i+1}U(x_{i+1}) = 0.$$

These three equations may be interpreted as a set of linear equations for the A_s. For a non-trivial solution we must have

$$\begin{vmatrix} P(x_{i-1}) & P(x_i) & P(x_{i+1}) \\ U(x_{i-1}) & U(x_i) & U(x_{i+1}) \\ V(x_{i-1}) & V(x_i) & V(x_{i+1}) \end{vmatrix} = 0. \tag{2.13}$$

Expanding this determinant by its first row gives

$$\begin{vmatrix} U(x_i) & U(x_{i+1}) \\ V(x_i) & V(x_{i+1}) \end{vmatrix} P(x_{i-1}) - \begin{vmatrix} U(x_{i-1}) & U(x_{i+1}) \\ V(x_{i-1}) & V(x_{i+1}) \end{vmatrix} P(x_i) + \begin{vmatrix} U(x_{i-1}) & U(x_i) \\ V(x_{i-1}) & V(x_i) \end{vmatrix} P(x_{i+1}) = 0, \tag{2.14}$$

and this is the desired equation.

To obtain an approximate difference equation we assume that between $x_{i-1} = x_i - h$, and $x_{i+1} = x_i + h$ the solutions of equation (2.11) may be adequately approximated by solutions of the equation

$$\frac{d^2P}{dx^2} + q(x_i, \lambda)P = 0. \tag{2.15}$$

If we now set $U(x) = \sin(\sqrt{[q(x_i, \lambda)](x - x_{i-1})})$, and $V(x) = \sin(\sqrt{[q(x_i, \lambda)](x - x_{i+1})})$, we find that equation (2.14) becomes

$$P(x_{i-1}) - 2\cos(h\sqrt{[q(x_i, \lambda)]})P(x_i) + P(x_{i+1}) = 0. \tag{2.16}$$

This equation has appeared several times in the literature (see, for example, Hersch (1958)). If $h\sqrt{q}$ is small enough it differs from the standard finite-difference approximation to (2.11) by terms which are $O(h^4q^2)$.

Formulae similar to equation (2.16) can be constructed by making different approximations to U and V. For example the W.K.B. method gives (assuming $q(x, \lambda) > 0$)

$$U = (4q(x, \lambda))^{-1/4} \sin(\eta(x) - \eta(x_{i-1})),$$
$$V = (4q(x, \lambda))^{-1/4} \sin(\eta(x) - \eta(x_{i+1})),$$
$$W_i = P(x_i)(4q(x_i, \lambda))^{1/4},$$

$$\sin(\eta(x_{i+1}) - \eta(x_i))W_{i-1} - \sin(\eta(x_{i+1}) - \eta(x_{i-1}))W_i + \sin(\eta(x_i) - \eta(x_{i-1}))W_{i+1} = 0. \tag{2.17}$$

Evaluating the integrals in (2.17) using the trapezoidal rule we have

$$\sin\left(\frac{h}{2}(\sqrt{q_{i+1}} + \sqrt{q_i})\right)W_{i-1} - \sin\left(\frac{h}{2}(\sqrt{q_{i+1}} + 2\sqrt{q_i} + \sqrt{q_{i-1}})\right)W_i + \sin\left(\frac{h}{2}(\sqrt{q_i} + \sqrt{q_{i-1}})\right)W_{i+1} = 0. \tag{2.18}$$

3. Iterative solution of the eigenvalue problem

In the examples discussed in the previous Section, finite-difference methods lead to the problem of solving equations having the form

$$\boldsymbol{A}(\lambda)\boldsymbol{V} = 0. \tag{3.1}$$

where the matrix $\boldsymbol{A}$ depends nonlinearly on λ.

For second-order equations with separated boundary conditions the matrix is also tridiagonal. This means that for any value of λ we can solve the problem

$$\boldsymbol{A}(\lambda)\boldsymbol{V} = \beta(\lambda)\boldsymbol{e}_p \tag{3.2}$$

by marching from each boundary and matching at a suitably chosen interior point x_p. Here $\boldsymbol{e}_p$ is a vector having one in the pth place and zeros elsewhere, while β depends on λ and on the choice of scale for the vector $\boldsymbol{V}$. The matching point is usually chosen to ensure a stable computation. For a more detailed treatment of the above points see Osborne (1962) and Fox (1960).

The eigenvalues of equation (3.1) are the zeros of $\beta(\lambda)$ defined in equation (3.2). To correct an approximate eigenvalue we can apply Newton's method to $\beta(\lambda)$. This requires us to know $d\beta/d\lambda$, and we find this by differentiating equation (3.2). This gives

$$A(\lambda)\frac{dV}{d\lambda} + \frac{dA}{d\lambda}V = \frac{d\beta}{d\lambda}e_p. \tag{3.3}$$

To solve equation (3.3) for $\frac{d\beta}{d\lambda}$ we have to make use of the method of scaling V in equation (3.2). For example, if A is symmetric (and a tridiagonal matrix whose off-diagonal elements are onesigned can always be made symmetric by premultiplying it by a diagonal matrix with positive elements) then we have, on taking the scalar product of equation (3.3) with V and using equation (3.2), that

$$\beta\left(\frac{dV}{d\lambda}\right)_p + V^T\frac{dA}{d\lambda}V = \frac{d\beta}{d\lambda}(V)_p. \tag{3.4}$$

If the scale has been fixed so that $(V)_p$ is independent of λ then $\left(\frac{dV}{d\lambda}\right)_p = 0$, and

$$\frac{d\beta}{d\lambda} = \frac{V^T\frac{dA}{d\lambda}V}{(V)_p}. \tag{3.5}$$

The improved value of λ is given by

$$\lambda \text{ improved} = \lambda - \frac{\beta(V)_p}{V^T\frac{dA}{d\lambda}V}. \tag{3.6}$$

The argument given above is identical with that used in Osborne (1962) for the special case when the elements of A depend linearly on λ. Note that equation (3.6) gives a correction to λ which is independent of the choice of scale. Thus the scaling assumed in the above derivation need not be carried out in the actual computation. This will be a feature of all the methods we discuss here. We will refer to the iteration summarized in equation (3.6) as iteration (A).

We now derive a more general iteration which we refer to as iteration (B). We let λ_i be the approximation to the eigenvalue found at the ith stage of the iteration, and during this stage we also calculate a vector x_i (we defer the exact specification of x_i until later). We now calculate a vector V_{i+1} from the equation

$$A(\lambda_i)V_{i+1} = \beta(\lambda_i)x_i \tag{3.7}$$

where, as before, the value of β is determined by requiring the vector V_{i+1} to be scaled according to some predetermined law. Varying λ_i keeping x_i fixed we see that $\beta(\lambda)$ vanishes at the eigenvalues of $A(\lambda)$. Thus again we apply Newton's method to $\beta(\lambda)$ to improve the approximate eigenvalue.

Differentiating equation (3.7) gives

$$A\frac{dV_{i+1}}{d\lambda} + \frac{dA}{d\lambda}V_{i+1} = \frac{d\beta}{d\lambda}x_i, \tag{3.8}$$

whence, using (3.7),

$$\frac{dV_{i+1}}{d\lambda} + A^{-1}\frac{dA}{d\lambda}V_{i+1} = \frac{1}{\beta}\frac{d\beta}{d\lambda}V_{i+1}. \tag{3.9}$$

If V_{i+1} is scaled so that one component (say the Pth) is fixed independent of λ then $\left(\frac{dV_{i+1}}{d\lambda}\right)_P = 0$, and we have

$$-\frac{\beta}{d\beta/d\lambda} = -\frac{(V_{i+1})_P}{\left(A^{-1}\frac{dA}{d\lambda}V_{i+1}\right)_P}. \tag{3.10}$$

Equation (3.10) gives us the desired correction to λ_i. However, we have still to settle the choice of the vector x_{i+1}. Two factors affect the approach of $\beta(\lambda)$ to zero and the accuracy with which V_{i+1} approximates to the eigenvector. These are (*a*) the nearness to singularity of the matrix $A(\lambda_i)$, and (*b*) the relative size of the component of x_i in the direction of the eigenvector. We attempt to maximize the second factor by linearizing the eigenvalue problem. We let $\bar{\lambda}$, $\bar{V}$ be approximations to the desired eigenvalue and the corresponding eigenvector. To first order we have

$$\left(A(\bar{\lambda}) + \frac{dA}{d\lambda}(\bar{\lambda})\Delta\lambda\right)(\bar{V} + \Delta V) = 0 \tag{3.11}$$

where $\Delta\lambda$ and the components of ΔV are assumed small. Ignoring second-order quantities we find that

$$\bar{V} + \Delta V = A^{-1}(\bar{\lambda})\frac{dA}{d\lambda}(\bar{\lambda})\bar{V} \tag{3.12}$$

where we have dropped a scale factor of $-\Delta\lambda$. If we define x_{i+1} by applying equation (3.12) with $\bar{\lambda} = \lambda_i$, $\bar{V} = V_{i+1}$ then x_{i+1} is just the vector that occurs in the denominator of equation (3.10).

We summarize iteration (B) in equation (3.13). We have

$$\left.\begin{aligned} A(\lambda_i)V_{i+1} &= \beta(\lambda_i)x_i \\ x_{i+1} &= A^{-1}(\lambda_i)\frac{dA}{d\lambda}(\lambda_i)V_{i+1} \\ \lambda_{i+1} &= \lambda_i - \frac{(V_{i+1})_P}{(x_{i+1})_P} \end{aligned}\right\}. \tag{3.13}$$

We note that a single step of the iteration requires a triangular factorization and two forward and back substitutions. We fix the value of P at each stage by selecting the component of x_{i+1} of maximum modulus. Again, as in iteration (A), it is not necessary to carry out any scaling explicitly except that required to keep the components of the successive vector iterates in range. When A depends linearly on λ a single step of our iteration is equivalent to two steps of inverse iteration plus a shift in the origin of λ. In special cases it is well known that it is desirable to maximize the component of x_i in the direction of the eigenvector.

Iteration (B) is formally of quite general application. However, when $A(\lambda)$ is symmetric it is possible to derive a formula which reduces the work involved per step by using a different scaling of the approximate eigenvector (in the special case where λ enters multiplying a positive definite matrix this formula reduces to one derived by Crandall (1951) who showed that it gives cubic convergence).

Here we scale V_{i+1} in equation (3.7) by requiring that

$$V_{i+1}^T S_i V_{i+1} = \text{constant} \tag{3.14}$$

where $S_i = \dfrac{dA}{d\lambda}(\lambda_i)$ is a constant matrix. We multiply equation (3.8) by V_{i+1}^T and use equation (3.7) and the symmetry of A. This gives

$$\beta x_i^T \frac{dV_{i+1}}{d\lambda} + V_{i+1}^T \frac{dA}{d\lambda} V_{i+1} = \frac{d\beta}{d\lambda} V_{i+1}^T x_i. \tag{3.15}$$

Differentiating equation (3.14) gives

$$V_{i+1}^T S_i \frac{dV_{i+1}}{d\lambda} = 0. \tag{3.16}$$

If we now set $x_i = \dfrac{dA}{d\lambda}(\lambda_i) V_i$, we have (using equation (3.16))

$$\beta x_i^T \frac{dV_{i+1}}{d\lambda} = \beta (V_i - V_{i+1})^T \frac{dA}{d\lambda} \frac{dV_{i+1}}{d\lambda}. \tag{3.17}$$

We can expect this term to be of second order as

(*a*) $\beta \to 0$, and (*b*) V_i, $V_{i+1} \to$ eigenvector.

If this term is ignored then equation (3.15) can be solved for $\dfrac{d\beta}{d\lambda}$. In this case the steps in the iteration are

$$A(\lambda_i) V_{i+1} = \beta(\lambda_i) x_i,$$

$$\lambda_{i+1} = \lambda_i - \frac{V_{i+1}^T x_i}{V_{i+1}^T \dfrac{dA}{d\lambda}(\lambda_i) V_{i+1}},$$

$$x_{i+1} = \frac{dA}{d\lambda}(\lambda_{i+1}) V_{i+1}. \tag{3.18}$$

We note that iteration (B) is formally applicable when the quantities appearing in equation (3.1) are complex valued, provided complex arithmetic is used. However, our methods have an interesting application to the real problem obtained by equating the real and imaginary parts of (3.1) to zero. We now have a two-parameter eigenvalue problem (corresponding to the real and imaginary parts of the complex eigenvalue), and two scale factors.

We write $\lambda = \lambda_1 + i\lambda_2$ and define the real and imaginary parts of the other quantities in (3.1) similarly. Separating real and imaginary parts leads us to the system

$$\begin{bmatrix} A_1(\lambda_1, \lambda_2) & -A_2(\lambda_1, \lambda_2) \\ A_2(\lambda_1, \lambda_2) & A_1(\lambda_1, \lambda_2) \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \end{bmatrix} = M\phi = 0. \tag{3.19}$$

We readily verify that the matrix $S(a, b) = \begin{bmatrix} aI & bI \\ -bI & aI \end{bmatrix}$ commutes with M for any values of a and b. Thus, if ϕ is a solution of (3.19), then so is $S(a, b)\phi$, and, in general, we may choose a and b so that any pair of elements $(i, n+j)$ of the solution vector ϕ take on prescribed values (α, β, say). The equations for a and b are

$$a(V_1)_i + b(V_2)_i = \alpha$$
$$-b(V_1)_j + a(V_2)_j = \beta$$

so that we require

$$\begin{vmatrix} (V_1)_i & (V_2)_i \\ -(V_1)_j & (V_2)_j \end{vmatrix} \neq 0.$$

We study the equation

$$M\phi = S(a, b)\psi. \tag{3.20}$$

Clearly the eigenvalues are zeros of $a(\lambda_1, \lambda_2) = b(\lambda_1, \lambda_2) = 0$. Holding ψ fixed and differentiating with respect to λ_1 we have

$$M \frac{\partial \phi}{\partial \lambda_1} + \frac{\partial M}{\partial \lambda_1} \phi = S\left(\frac{\partial a}{\partial \lambda_1}, \frac{\partial b}{\partial \lambda_1}\right) \psi$$

whence

$$\frac{\partial \phi}{\partial \lambda_1} + M^{-1} \frac{\partial M}{\partial \lambda_1} \phi = S\left(\frac{\partial a}{\partial \lambda_1}, \frac{\partial b}{\partial \lambda_1}\right) M^{-1} \psi \tag{3.21}$$

(as a matrix which commutes with M commutes with M^{-1}). Writing $\S^{(1)} = M^{-1} \dfrac{\partial M}{\partial \lambda_1} \phi$ and using (3.20) gives

$$\frac{\partial \phi}{\partial \lambda_1} + \S^{(1)} = S\left(\frac{\partial a}{\partial \lambda_1}, \frac{\partial b}{\partial \lambda_1}\right) S(a, b)^{-1} \phi. \tag{3.22}$$

We scale so that $(\phi)_i$, $(\phi)_{n+j}$ are independent of λ_1, λ_2. Equating the i, and $n+j$ components of $\dfrac{\partial \phi}{\partial \lambda_1}$ to zero in (3.22) gives

$$\begin{bmatrix} (\S^{(1)})_i \\ (\S^{(1)})_{n+j} \end{bmatrix} (a^2 + b^2)$$

$$= \begin{bmatrix} a(V_1)_i - b(V_2)_i & b(V_1)_i + a(V_2)_i \\ b(V_1)_j + a(V_2)_j & -a(V_1)_j + b(V_2)_j \end{bmatrix} \begin{bmatrix} \dfrac{\partial a}{\partial \lambda_1} \\ \dfrac{\partial b}{\partial \lambda_1} \end{bmatrix}. \tag{3.23}$$

We carry through a similar calculation differentiating (3.20) with respect to λ_2. We set $\S^{(2)} = M^{-1} \dfrac{\partial M}{\partial \lambda_2} \phi$, and we combine the results with equation (3.23) to give

$$\begin{bmatrix} (\S^{(1)})_i & (\S^{(2)})_i \\ (\S^{(1)})_{n+j} & (\S^{(2)})_{n+j} \end{bmatrix} (a^2 + b^2)$$

$$= \begin{bmatrix} a(V_1)_i - b(V_2)_i & b(V_1)_i + a(V_2)_i \\ b(V_1)_j + a(V_2)_j & -a(V_1)_j + b(V_2)_j \end{bmatrix} \begin{bmatrix} \dfrac{\partial a}{\partial \lambda_1} & \dfrac{\partial a}{\partial \lambda_2} \\ \dfrac{\partial b}{\partial \lambda_1} & \dfrac{\partial b}{\partial \lambda_2} \end{bmatrix} \tag{3.24}$$

The corrections $\Delta\lambda_1$, $\Delta\lambda_2$ are found from the equation

$$\begin{bmatrix} \frac{\partial a}{\partial \lambda_1} & \frac{\partial a}{\partial \lambda_2} \\ \frac{\partial b}{\partial \lambda_1} & \frac{\partial b}{\partial \lambda_2} \end{bmatrix} \begin{bmatrix} \Delta\lambda_1 \\ \Delta\lambda_2 \end{bmatrix} + \begin{bmatrix} a \\ b \end{bmatrix} = 0. \tag{3.25}$$

We eliminate the partial derivatives with respect to λ_1 and λ_2 between equations (3.24) and (3.25), and solve the resulting equation for $\begin{bmatrix} \Delta\lambda_1 \\ \Delta\lambda_2 \end{bmatrix}$. We find

$$\begin{bmatrix} \Delta\lambda_1 \\ \Delta\lambda_2 \end{bmatrix} = - \begin{bmatrix} (\S^{(1)})_i & (\S^{(2)})_i \\ (\S^{(1)})_{n+j} & (\S^{(2)})_{n+j} \end{bmatrix}^{-1} \begin{bmatrix} (V_1)_i \\ (V_2)_j \end{bmatrix}. \tag{3.26}$$

Arguing as before we take for the next step of the iteration the vector ψ defined by the equation

$$\psi = \Delta\lambda_1 \S^{(1)} + \Delta\lambda_2 \S^{(2)}. \tag{3.27}$$

4. Numerical examples

We summarize here numerical results obtained by applying the procedures derived in the previous Section to problems of the type considered in Section 2.

In our first example the standard finite-difference formulae are used to approximate to the eigenvalue problem

$$\frac{d}{dx}\left\{(1 - x^2)\frac{dP}{dx}\right\} + \lambda P = 0$$

$$P(-1) \text{ finite}, \quad P(0) = 0. \tag{4.1}$$

At the singular point $x = -1$ the equation is approximated by the formula derived in Section 2 (equation (2.5)). We have used both iteration (A) and iteration (B) to calculate approximations to the first few eigenvalues, and the results of our computation of the first, second, and fourth eigenvalues are given in Table 4.1.

We remark that apart from the first eigenvalue, which is a special case, iteration (B) seems superior to iteration (A). A feature of iteration (B) which has been borne out in further numerical experiments is the sudden large reduction in the magnitude of $\Delta\lambda$. This suggests that it has better than second-order convergence. Results very similar in character to those displayed in Table 4.1 have been obtained by Mr. William McLewin of Reading University for an eigenvalue problem with one boundary at ∞. He treats this boundary point in a manner similar to that described in Section 2.

In our second example we have used iteration (B) to solve the finite-difference approximations of Hersch type (equations (2.16) and (2.18)) to the eigenvalue problems

$$\frac{d^2P}{dx^2} + (\lambda + x)P = 0,$$

$$P(0) = P(1) = 0, \tag{4.2}$$

Table 4.1

ITERATIONS	A		B	
	λ	$\Delta\lambda$	λ	$\Delta\lambda$
accurate $\lambda = 2$, $h =$ ·04, approximate $\lambda = 2$.				
	1·75	·25497217	1·75	·24248686
	2·0049722	— ·00497021	1·9924869	·00750802
	2·0000020	— ·00000200	1·9999949	·00000523
	2·0000000	·00000007	2·0000001	— ·00000014
	2·0000000		2·0000000	
accurate $\lambda = 12$, $h =$ ·04, approximate $\lambda = 12{\cdot}000067$				
	10	1·5698286	10	2·3299555
	11·569829	·41911135	12·329956	— ·32988507
	11·988940	·01112123	12·000070	— ·00000243
	12·000061	·00000604	12·000068	— ·00000089
	12·000067	·00000033	12·000067	
	12·000067			
accurate $\lambda = 56$, $h =$ ·02, approximate $\lambda = 56{\cdot}009953$				
	60	—2·2350126	60	—4·1201602
	57·764987	—1·4672299	55·879840	·13011891
	56·297757	— ·28121636	56·009958	— ·00000515
	56·016541	— ·00658511	56·009953	— ·00000138
	56·009956	— ·00000176	56·009952	— ·00000007
	56·009954	— ·00000071	56·009952	
	56·009954			

and

$$\frac{d^2P}{dx^2} + \left\{\frac{9\lambda}{16}(1 + x^2)^2 + \frac{27x}{64}\left(1 + \frac{x^2}{3}\right)(1 + x^2)^2 + \frac{1 - 2x^2}{(1 + x^2)^2}\right\}P = 0,$$

$$P(0) = P(1) = 0. \tag{4.3}$$

Equations (4.2) and (4.3) can be transformed into each other by suitably transforming both independent and dependent variables so that they have the same eigenvalues. It is not difficult to show (from equation (4.2)) that these eigenvalues satisfy

$$\lambda_p = p^2\pi^2 - \tfrac{1}{2} + O(1/p^2). \tag{4.4}$$

Equation (4.4) provides a convenient check on the accuracy of our difference approximations. As an additional check we computed some of the lower eigenvalues using a different numerical procedure.

In our numerical working we took $h = 1/26$ and attempted to evaluate the first 25 eigenvalues starting with the approximations $\lambda_i = (3{\cdot}142i)^2$. This was easily accomplished using equation (2.16) to approximate to equation (4.2). However, when the approximation (2.16) was applied to equation (4.3) it failed to converge at the 21st eigenvalue. At this stage the approximate eigenvalues are no longer close to the exact

Table 4.2

n	$n^2\pi^2 - \frac{1}{2}$	HERSCH METHOD EQUATION (4.2)		HERSCH METHOD EQUATION (4.3)		HERSCH (W.K.B.) METHOD EQUATION (4.3)	
		λ	$\Delta\lambda$	λ	$\Delta\lambda$	λ	$\Delta\lambda$
		9·8721640	— ·50462505	9·8721640	— ·50373174	9·8721640	— ·92773141
		9·3675389	·00095094	9·3684323	·00008710	8·9444326	— ·03906426
		9·3684899	·00000314	9·3685193	— ·00000093	8·9053683	— ·00008218
1	9·3696044	9·3684931		9·3685184		8·9052861	·00000196
						8·9052881	
		39·488656	—1·6187659	39·488656	— ·52423552	39·488656	—1·0038301
		37·869890	1·1067916	38·964420	·01466074	38·484826	·01552393
		38·976682	·00204837	38·979081	·00000130	38·500350	·00000162
		38·978730	— ·00000088	38·979083		38·500351	
2	38·978418	38·978729					
		5686·3664	36·919542			5686·3664	—4·3156467
		5723·2860	—39·690534			5682·0508	— ·22302597
		5683·5954	·79650682			5681·8278	·00099366
		5684·3920	·00034420			5681·8288	
24	5684·3921	5684·3923					
		6170·1025	—2·1134689			6170·1025	—41·326951
		6167·9890	·01421548			6128·7755	28·542241
		6168·0032	— ·00001820			6157·3178	8·1102630
25	6168·0028	6168·0032				6165·4280	— ·17024050
						6165·2578	— ·00012516
						6165·2577	

values. This led us to investigate the approximation to equation (4.3) provided by the W.K.B. modification (equation (2.18)). Here we found 25 eigenvalues. However, although the higher eigenvalues are tolerably accurate the first few are not good. We present some of the numerical results in Table 4.2. They illustrate the convergence of the iterative procedure while indicating some interesting problems concerning the degree of approximation to the differential equation.

As in our first example, iteration (B) provides a powerful method for refining an approximate eigenvalue. An interesting feature of the iterations in the approximation to equation (4.2) by equation (2.16) is the erroneous first value of $\Delta\lambda$ for the eigenvalues of even order. The reason for this is that we set every element of the starting vector x_0 equal to 1, making it nearly orthogonal to the even-order eigenvectors. This illustrates the importance of having a large component of the x_i in the direction of the eigenvector.

A program has been written to implement the iteration for finding complex eigenvalues suggested in Section 3. This program has been checked on the Atlas computer using a simple test matrix, and once again very rapid convergence has been obtained.

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