BIT 24 (1984), 401–412

ON THE CORRECTION OF FINITE DIFFERENCE EIGENVALUE APPROXIMATIONS FOR STURM-LIOUVILLE PROBLEMS WITH GENERAL BOUNDARY CONDITIONS

R.S. ANDERSSEN and F. R. DE HOOG
CSIRO Division of Mathematics and Statistics, GPO Box 1965, Canberra City, ACT 2601, Australia.

Dedicated to Germund Dahlquist on the occasion of his 60th birthday.

Abstract.

When finite difference and finite element methods are used to approximate continuous (differential) eigenvalue problems, the resulting algebraic eigenvalues only yield accurate estimates for the fundamental and first few harmonics. One way around this difficulty would be to estimate the error between the differential and algebraic eigenvalues by some independent procedure and then use it to correct the algebraic eigenvalues. Such an estimate has been derived by Paine, de Hoog and Anderssen for the Liouville normal form with Dirichlet boundary conditions. In this paper, we extend their result to the Liouville normal form with general boundary conditions.

1. Introduction.

Because it is representative of a wide class of continuous eigenvalue problems, we work in this paper with the canonical Liouville normal form

$$-y''+qy = \lambda y, \qquad q = q(x), \qquad y = y(x), \qquad 0 \leqslant x \leqslant \pi, \tag{1}$$

$$\alpha_1 y'(0)-\alpha_2 y(0) = 0, \qquad \beta_1 y'(\pi)+\beta_2 y(\pi) = 0. \tag{2}$$

In fact, from both a theoretical and a numerical point of view, the analysis of an eigenvalue problem as its Liouville normal form has considerable advantages (cf. [8]). However, the transformation to Liouville normal form must often be performed numerically and introduces its own computational difficulties (cf. [5]). This aspect will not be pursued here.

When discrete (finite difference and finite element) eigenvalue problems are used to approximate continuous (differential) eigenvalue problems, it is not only necessary to prove that the numerical method used to solve the discrete problem is efficient and accurate, but also necessary to establish that the exact eigenvalues of the discrete problem itself yield accurate estimates of the

Received January 1984. Revised May 1984.

corresponding eigenvalues of the continuous problem. In fact, because accurate and reliable methods can be constructed for the solution of the discrete (algebraic) eigenvalue problems (cf. [10], Chapter 2), the accuracy of the approximate eigenvalues obtained is limited by the accuracy with which the exact eigenvalues of the discrete problem approximate the corresponding eigenvalues of the continuous problem.

For example, consider the use of finite difference methods for the simplest of all Sturm-Liouville problems

$$-w'' = \eta w, \qquad w(0) = w(\pi) = 0. \tag{3}$$

Its exact eigenvalues and eigenfunctions are given respectively by

$$\eta_k = k^2, \qquad w_k = \sin(kx), \qquad k = 1, 2, \ldots \tag{4}$$

If, at the internal grid points of the uniform grid

$$G = \{x_i; x_i = ih,\ i = 0, 1, 2, \ldots, n+1,\ h = \pi/(n+1)\},$$

the second derivative in (3) is approximated using central differences, the following algebraic eigenvalue problem is obtained

$$-A\tilde{w} = \eta^{(n)}\tilde{w}$$

with

$$A = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & \cdot & \cdot & \cdot \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix}$$

and $\tilde{w} = [\tilde{w}_1, \tilde{w}_2, \ldots, \tilde{w}_n]^T$, $\tilde{w}_i \simeq w_i = w(x_i)$, $i = 1, 2, \ldots, n$. For notational convenience, the explicit dependence of the algebraic eigenvectors on n will be suppressed. This problem can be solved without error since the eigenvalues $\eta_k^{(n)}$ and the corresponding eigenfunctions $\tilde{w}_k$ are known to be

$$\eta_k^{(n)} = 4\sin^2(kh/2)/h^2$$

and

$$\tilde{w}_k = [\sin kh, \sin 2kh, \ldots, \sin nkh]^T.$$

Thus the error

$$e_k^{(n)} = \eta_k - \eta_k^{(n)} = O(k^4/(n+1)^2) = O(k^4h^2) \tag{5}$$

is due solely to the use of finite difference methods in the approximation of (3). Its $O(k^4h^2)$ behaviour clearly establishes that the accuracy of the approximations $\eta_k^{(n)}$ deteriorates rapidly as k increases.

This dependence on k, which will always be made explicit in the present paper, verifies that the accuracy of the approximate eigenvalues is controlled strongly by the form chosen for the discrete problem and that, when finite difference and finite element methods are used, the resulting algebraic eigenvalues will only yield accurate estimates for the fundamental and first few harmonics.

This does not negate the use of finite difference methods when approximations to the first m eigenvalues of a differential eigenvalue problem are required with $m \gg 1$. But, it does imply that some redundancy must be built into the algebraic eigenvalue problem used to construct the approximations before accurate estimates will be generated. A common technique, used by engineers, geophysicists and others, is to construct the discrete problem for $n = lm$, with $l \gg 1$, but only calculate its first m eigenvalues (cf. [10], §§2–2, 15–12).

From a computational and numerical analysis point of view, such a procedure represents an obtuse way to calculate differential eigenvalues. An alternative approach is to work directly with the given differential eigenvalue problem to obtain estimates which have errors that can be bounded independently of k. There are a number of ways in which this can be done. In the classical approach, the Sturm–Liouville problem (or Liouville normal form) is replaced by a first order differential equation which is solved using shooting methods. Included in this class are the Prüfer phase methods (cf. [5], and [6] for a summary). In a more recent approach, pursued with considerable success by a number of authors including Pruess [11], [12] and Paine and de Hoog [8], a simpler problem is constructed by replacing the coefficients in the Sturm–Liouville problem (or Liouville normal form) by piecewise constants. In fact, Paine and de Hoog [8] have clearly established the numerical advantages of the Liouville normal form by showing that, when this approach is applied to (1) and (2), $O(h^2)$ accurate appoximations to the eigenvalues are generated. Summaries of the various methods which have been used, along with error estimates for the corresponding appoximate eigenvalues, is given in [6] and [2]. The latter paper discusses the use of comparison theorems to construct computable error bounds. Subsequently, Paine and Andrew [7] have derived $O(h^2)$ methods of this type.

Another way around the difficulty would be to estimate the error between the differential and algebraic eigenvalues by some independent procedure and then use it to correct the algebraic eigenvalues.

In 1981, Paine, de Hoog and Anderssen derived such an estimate for the Liouville normal form with Dirichlet boundary conditions

(6) $$-v''+qv = \theta v, \qquad q = q(x), \qquad v = v(x), \qquad 0 < x < \pi,$$

(7) $$v(0) = v(\pi) = 0.$$

They showed that

(8) $$\theta_k - \theta_k^{(n)} = e_k^{(n)} + O(kh^2), \qquad 1 < k \leqslant \alpha n,\ \alpha < 1,$$

where the $\theta_k^{(n)}$ correspond to the central difference eigenvalues of (6) and (7) on the uniform grid G and therefore satisfy

$$(-A+Q)\tilde{v} = \theta^{(n)}\tilde{v}, \qquad \tilde{v} = [\tilde{v}_1, \tilde{v}_2, \ldots, \tilde{v}_n]^T,$$

where $Q = \operatorname{diag}(q_1, q_2, \ldots, q_n)$, and $\tilde{v}_i \simeq v_i = v(x_i)$, $q_i = q(x_i)$, $i = 1, 2, \ldots, n$.
This leads naturally to the correction formula

$$\tilde{\theta}_k^{(n)} = \theta_k^{(n)} + e_k^{(n)}, \quad k = 1, 2, \ldots, n,\ n = 1, 2, \ldots.$$

The derivation of (8) is greatly simplified because the boundary conditions are Dirichlet and the exact value of $e_k^{(n)}$ of (5) is known. In this paper we show that similar results to (8) hold for the Liouville normal form (1) and (2). The central difference eigenvalues $\lambda_k^{(n)}$, $k = 0, 1, 2, \ldots, n$, of (1) and (2) satisfy, on the augmented grid

$$G^* = \{x_j; x_j = jh, j = -1, 0, 1, \ldots, n, n+1,\ h = \pi/n\},$$

the following algebraic system

(9) $$(-L+Q)\tilde{y} = \lambda^{(n)}\tilde{y}, \qquad \tilde{y} = [\tilde{y}_0, \tilde{y}_1, \ldots, \tilde{y}_n]^T$$

with

$$L = h^{-2}\begin{bmatrix} -2 & p & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots \\ & & 1 & -2 & 1 \\ & & & q & -2 \end{bmatrix}; \quad \begin{array}{l} p = 2\alpha_1/(\alpha_1 + h\alpha_2) \\ q = 2\beta_1/(\beta_1 + h\beta_2) \end{array}$$

and $\tilde{y}_j \simeq y_j = y(x_j)$, $j = 0, 1, \ldots, n$, when the boundary conditions (2) are approximated by the following finite difference formulas

$$\alpha_1(\tilde{y}_1-\tilde{y}_{-1})/2h-\alpha_2\tilde{y}_0 = 0,$$

and
$$\beta_1(\tilde{y}_{n+1}-\tilde{y}_{n-1})/2h+\beta_2\tilde{y}_n = 0.$$

For the Liouville normal form (1) and (2), the counterpart of (3) takes the form

$$(10) \qquad -u'' = \gamma u, \qquad u = u(x),$$

$$(11) \qquad \alpha_1 u'(0)-\alpha_2 u(0) = 0, \qquad \beta_1 u'(\pi)-\beta_2 u(\pi) = 0.$$

The central difference eigenvalues of (10) and (11) corresponding to the $\lambda^{(n)}$ of (9) are therefore defined by

$$(12) \qquad -L\tilde{\boldsymbol{u}} = \gamma^{(n)}\tilde{\boldsymbol{u}}, \qquad \tilde{\boldsymbol{u}} = [\tilde{u}_0, \tilde{u}_1, \ldots, \tilde{u}_n]^T,$$

with $\tilde{u}_i \simeq u_i = u(x_i)$, $i = 0, 1, \ldots, n$.

The main result of this paper can now be stated.

THEOREM. *Under the assumption that $q''(x)$ is continuous on $[0, \pi]$, it follows that there exists an $\alpha < 1$ which is independent of n such that*

$$(13) \qquad \lambda_k-\lambda_k^{(n)} = \varepsilon_k^{(n)}+O(h^2), \qquad 1 < k \leqslant \alpha n,$$

with
$$\varepsilon_k^{(n)} = \gamma_k-\gamma_k^{(n)}.$$

It will be proved in Section 2. It leads naturally to the correction procedure

$$(14) \qquad \bar{\lambda}_k^{(n)} = \lambda_k^{(n)}+\varepsilon_k^{(n)}, \qquad k = 0, 1, 2, \ldots, n.$$

In establishing the relationship between $\lambda_k-\lambda_k^{(n)}$ and $\gamma_k-\gamma_k^{(n)}$, asymptotic expansions are derived for various quantities including λ_k and $\lambda_k^{(n)}$. In fact, we find that, when $\alpha_1 = \beta_1 = 0$,

$$\lambda_k = k^2+O(1)$$

and
$$\lambda_k^{(n)} = 4\sin^2(kh/2)/h^2+O(1).$$

But, the first term in the difference between these two asymptotic expansions is just the correction $e_k^{(n)}$ of (5) derived and used by Paine, de Hoog and Anderssen [9]. This suggests that the difference

$$\tilde{\varepsilon}_k^{(n)} = \tilde{\lambda}_k-\tilde{\lambda}_k^{(n)}$$

between the leading terms in the asymptotic expansions for the continuous and discrete problems

$$\lambda_k = \tilde{\lambda}_k + O(k^{-m}), \tag{15}$$

and

$$\lambda_k^{(n)} = \tilde{\lambda}_k^{(n)} + O(k^{-m}),$$

respectively, can also be used to correct the algebraic eigenvalue approximations; namely,

$$\tilde{\lambda}_k^{(n)} = \lambda_k^{(n)} + \tilde{\varepsilon}_k^{(n)}, \qquad k = 0, 1, 2, \ldots, n, \qquad n = 1, 2, \ldots \tag{16}$$

The case $m = 3$ is discussed in section 2. Implementation of the correction procedures and numerical verification of the results are examined in section 3.

2. The estimate $\lambda_k - \lambda_k^{(n)} = \varepsilon_k^{(n)} + O(h^2)$.

The essence of the proof is straight-forward once appropriate asymptotic formulas are available, though the details are technically awkward (cf. Anderssen and de Hoog [1]). Those used in the present examination were derived in [1] and [3].

Throughout the remainder of this paper, we shall make the assumption that

$$\int_0^\pi q(x)\,dx = 0.$$

This simplifies the proof at crucial stages without affecting their generality, since (cf. [4]) the only contribution that a non-zero value of this integral makes to the λ_k is a translation.

For notational convenience, the dependence of λ_k, $\lambda_k^{(n)}$, γ_k, $\gamma_k^{(n)}$, $\tilde{\lambda}_k$, $\tilde{\lambda}_k^{(n)}$, etc. on k will often be suppressed in the sequel when there is no ambiguity of meaning.

Because there is a sign redundancy in the boundary conditions (2), we shall assume that

$$\alpha_1 \geqslant 0 \quad \text{and} \quad \beta_1 \geqslant 0.$$

In addition, we introduce the notation

$$q_1(x) = \int_0^x q(\tau)\,d\tau. \tag{17}$$

Logically, the derivation of the results above involves two basically distinct steps:

1. Formal estimates of the error $\lambda-\lambda^{(n)}$ in terms of $\tilde{\lambda}-\tilde{\lambda}^{(n)}$, and in terms of $\gamma-\gamma^{(n)}$.

2. Construction of explicit estimates for $\tilde{\lambda}-\tilde{\lambda}^{(n)}$ and for $\gamma-\gamma^{(n)}$ which can be used to apply the corrections (14) and (16).

Technically, the explicit estimates of the second step are needed to prove the estimates of the first.

The construction of such explicit formulas depends crucially on the use of appropriate asymptotic formulas for the eigenvalues λ, $\lambda^{(n)}$, γ and $\gamma^{(n)}$ of (1)–(2), (9), (10)–(11) and (12), respectively, the eigenfunction $y(x)$ and the eigenvector $\tilde{y} = (\tilde{y}_0, \tilde{y}_1, \ldots, \tilde{y}_n)^T$. It is these formulas which are derived in [3]. In general, they are only valid for $1 < k \leqslant \alpha n$, with $\alpha < 1$ and independent of n.

Asymptotic Formula for γ_k. For the Liouville normal form (10)–(11),

$$\gamma = \mu^2, \qquad u(x) = \cos(\mu x+\phi),$$

where $\phi = O(k^{-1})$, $\mu = O(k)$ and μ satisfies the following fixed point formula

$$\mu = k-1+\{\sin^{-1}(\beta_2/(\beta_2^2+\beta_1^2\mu^2)^{1/2})+\sin^{-1}(\alpha_2/(\alpha_2^2+\alpha_1^2\mu^2)^{1/2}\}/\pi.$$

Asymptotic Formula for $\gamma_k^{(n)}$. For the discrete problem (12),

$$\gamma^{(n)} = 4\sin^2(\tilde{\mu}h/2)/h^2, \qquad \tilde{u}_j = \cos(\tilde{\mu}x_j+\tilde{\phi}), \qquad j = 0, 1, \ldots, n,$$

where $\tilde{\phi} = O(k^{-1})$, $\tilde{\mu} = O(k^{-1})$ and $\tilde{\mu}$ satisfies the following fixed point formula

$$\tilde{\mu} = k-1+\{\sin^{-1}(\beta_2/(\beta_2^2+\beta_1^2\hat{\mu}^2)^{1/2})+\sin^{-1}(\alpha_2/(\alpha_2^2+\alpha_1^2\hat{\mu}^2)^{1/2})\}/\pi,$$

with

$$\hat{\mu} = \sin(\tilde{\mu}h)/h.$$

Asymptotic Formula for $y(x)$. For the Liouville normal form (1)–(2),

$$y = \cos(\mu x+\phi)+\frac{1}{2\mu}\sin(\mu x+\phi)\,q_1(x)+\frac{1}{4\mu^2}\{\cos(\mu x+\phi)q(x)$$

$$-\cos(\mu x-\phi)\,q(0)-\tfrac{1}{2}\cos(\mu x+\phi)q_1^2(x)\}+O(k^{-3})$$

with $q(x)$, $q_1(x)$, μ and ϕ defined above.

Asymptotic Formula for $\tilde{y}_j$. For the discrete problem (9)

(18) $$\tilde{y}_j = \cos(\tilde{\mu}x_j+\tilde{\phi})+\frac{h}{\sin\tilde{\mu}h}\sin(\tilde{\mu}x_j+\tilde{\phi})q_1(x_j)$$

$$+\tfrac{1}{4}\left(\frac{h}{\sin\tilde{\mu}h}\right)^2\{\cos(\tilde{\mu}h)[q(x_j)\cos(\tilde{\mu}x_j+\tilde{\Phi})-q(0)\cos(\tilde{\mu}x_j-\tilde{\Phi})]$$

$$-\tfrac{1}{2}\cos(\tilde{\mu}x_j+\tilde{\Phi})q_1^2(x_j)\}+O(k^{-3}),$$

with $q(x)$, $q_1(x)$, $\tilde{\mu}$ and $\tilde{\Phi}$ defined above.

Asymptotic Formula for $\lambda_k^{(n)}$. For the discrete problem (9), $\lambda_k^{(n)} = \tilde{\lambda}_k^{(n)}+O(k^{-3})$ with

$$\tilde{\lambda}_k^{(n)} = \gamma_k^{(n)}+\frac{1}{\pi}\left(\frac{h^2}{12}(q'(\pi)-q'(0))+\frac{h\cot\tilde{\mu}h}{2}\{q(\pi)\beta+q(0)\alpha\}\right. \tag{19}$$

$$\left.+\frac{h^2}{4\sin^2\tilde{\mu}h}\{q'(\pi)\bar{\beta}-q'(0)\bar{\alpha}\}+\tfrac{1}{4}\left(\frac{h}{\sin\tilde{\mu}h}\right)^2\cos\tilde{\mu}h\int_0^\pi q^2(x)\,dx\right),$$

where
$$\alpha = 2\alpha_1\alpha_2(\sin\tilde{\mu}h/h)\{\alpha_2^2+\alpha_1^2(\sin\tilde{\mu}h/h)^2\},$$

$$\beta = 2\beta_1\beta_2(\sin\tilde{\mu}h/h/\{\beta_2^2+\beta_1^2(\sin\tilde{\mu}h/h)^2\},$$

$$\bar{\alpha} = \{\alpha_1^2\sin^2(\tilde{\mu}h)/h^2-\alpha_2^2/\{\alpha_2^2+\alpha_1^2\sin^2(\tilde{\mu}h)/h^2\},$$

and
$$\bar{\beta} = \{\beta_1^2\sin^2(\tilde{\mu}h)/h^2-\beta_2^2\}/\{\beta_2^2+\beta_1^2\sin^2(\tilde{\mu}h)/h^2\},$$

with $q(x)$, $q_1(x)$, $\tilde{\mu}$ and $\tilde{\Phi}$ defined above.

Asymptotic Formula for λ_k. For the continuous Liouville normal form (1)–(2), the required value for $\tilde{\lambda}_k$ of (15) is obtained by taking the limit as $h\to 0$ in the formula (19) for $\tilde{\lambda}_k^{(n)}$

$$\tilde{\lambda}_k = \gamma_k+\frac{1}{\pi}\left(\frac{1}{2\mu_k}\{q(\pi)\hat{\beta}+q(0)\hat{\alpha}\}+\frac{1}{4\mu_k^2}\{q'(\pi)\hat{\hat{\beta}}-q'(0)\hat{\hat{\alpha}}\}\right. \tag{20}$$

$$\left.+\frac{1}{4\mu_k^2}\int_0^\pi q^2(x)\,dx\right),$$

where
$$\hat{\alpha} = 2\alpha_1\alpha_2\mu_k/\{\alpha_2^2+\alpha_1^2\mu_k^2\},$$

$$\hat{\beta} = 2\beta_1\beta_2\mu_k/\{\beta_2^2+\beta_1^2\mu_k^2\},$$

$$\hat{\hat{\alpha}} = \{\alpha_1^2\mu_k^2-\alpha_2^2\}/\{\alpha_2^2+\alpha_1^2\mu_k^2\},$$

and
$$\hat{\hat{\beta}} = \{\beta_1^2\mu_k^2-\beta_2^2\}/\{\beta_2^2+\beta_1^2\mu_k^2\},$$

with $q(x)$ and μ_k defined above.

PROOF OF (13). Because the asymptotic formulas above are $O(k^{-3})$ estimates, which do not depend on h, it is necessary to go to the explicit relationship between the continuous problem (1) and (2) and the discrete problem (9), which does depend on h, before the required $O(h^2)$ estimate of (13) can be derived. It is this aspect which makes the proof of (13) technically awkward.

From (1) and (9), it follows that

$$-y_j'' + q_j y_j = \lambda_k y_j, \qquad j = 0, 1, 2, \ldots, n, \qquad \text{and} \tag{21}$$

$$-\delta^2 \tilde{y}_j/h^2 + q_j \tilde{y}_j = \lambda_k^{(n)} \tilde{y}_j, \qquad j = 0, 1, 2, \ldots, n, \tag{22}$$

where δ^2 denotes the central difference operator $\delta^2 \tilde{y}_j = \tilde{y}_{j+1} - 2\tilde{y}_j + \tilde{y}_{j-1}$.

Together, (21) and (22) yield

$$(\lambda_k - \lambda_k^{(n)}) h \sum_{j=0}^{n}{}' \tilde{y}_j y_j = h \sum_{j=0}^{n}{}' \{y_j \delta^2 \tilde{y}_j/h^2 - \tilde{y}_j y_j''\}, \tag{23}$$

where the following summation convention has been used

$$\sum_{j=0}^{n}{}' \theta_j = \tfrac{1}{2}\theta_0 + \sum_{j=1}^{n-1} \theta_j + \tfrac{1}{2}\theta_n.$$

On using the asymptotic expansion

$$\tilde{y}_j = \tilde{c}_j + \bar{\varepsilon}_j, \qquad \tilde{c}_j = \cos(\tilde{\mu}_k x_j + \tilde{\Phi}), \qquad \bar{\varepsilon}_j = O(k^{-1}),$$

which follows from (18), identity (23) becomes

$$(\lambda_k - \lambda_k^{(n)}) h \sum_{j=0}^{n}{}' \tilde{y}_j y_j = h \sum_{j=0}^{n}{}' \{\delta^2 \tilde{c}_j/h^2 + \mu_k^2 \tilde{c}_j\} y_j \tag{24}$$

$$-h \sum_{j=0}^{n}{}' \{\mu_k^2 y_j + y_j''\} \tilde{c}_j + h \sum_{j=0}^{n}{}' \{\delta^2 \bar{\varepsilon}_j y_j/h^2 - \bar{\varepsilon}_j y_j''\}.$$

Through the repeated use of the asymptotic formulas above as well as estimates derived from the trapezoidal integration rule (cf. [1] for a more detailed discussion) individual estimates are derived for the three terms on the right hand side of (24). Together they yield

$$(\lambda_k - \lambda_k^{(n)}) h \sum_{j=0}^{n}{}' \tilde{y}_j y_j = (\gamma_k - \gamma_k^{(n)}) h \sum_{j=0}^{n}{}' \tilde{c}_y y_j + (\gamma_k - \hat{\gamma}_k) h \sum_{j=0}^{n}{}' \bar{\varepsilon}_j y_j \tag{25}$$

$$+ I(y) + R_1(y) + R_2(y) + O(h^2),$$

with $\hat{\gamma}_k = 4\sin^2(\mu_k h/2)/h^2$, $I(y) = (\tilde{\mu}_k^2-\gamma_k)\int_0^\pi \cos(\tilde{\mu}_k x+\tilde{\Phi})y(x)\,dx$,

$$R_1(y) = -\{y'(\pi)\cos(\tilde{\mu}_k\pi+\tilde{\Phi})+y(\pi)\tilde{\mu}_k\sin(\tilde{\mu}_k\pi+\tilde{\Phi})\}$$

$$+y(\pi)\left(\frac{\bar{\varepsilon}_{n+1}-\bar{\varepsilon}_{n-1}}{2h}\right)-\bar{\varepsilon}_n\left(\frac{y_{n+1}-y_n}{2h}\right), \text{ and}$$

$$R_2(y) = y'(0)\cos\tilde{\Phi}+y(0)\tilde{\mu}_k\sin\tilde{\Phi}-y(0)\frac{(\bar{\varepsilon}_1-\bar{\varepsilon}_{-1})}{2h}-\bar{\varepsilon}_0\frac{(y_1-y_{-1})}{2h}.$$

Further manipulation of various properties of $\tilde{\mu}_k$, γ_k, $\hat{\gamma}_k$, and the asymptotic formulas, then yield the following estimates for the terms in (25):

$$(\gamma_k-\gamma_k^{(n)})h\sum_{j=0}^{n}{}' \tilde{\varepsilon}_j y_j+(\gamma_k-\hat{\gamma}_k)h\sum_{j=0}^{n}{}' \varepsilon_j y_j = (\gamma_k-\gamma_k^{(n)})h\sum_{j=0}^{n}{}' \tilde{y}_j y_j+O(h^2),$$

$$I(y)+R_1(y)+R_2(y) = O(h^2).$$

Substitution of these two results into (25) yields

$$(\lambda_k-\lambda_k^{(n)})h\sum_{j=0}^{n}{}' \tilde{y}_j y_j = (\gamma_k-\gamma_k^{(n)})h\sum_{j=0}^{n}{}' \tilde{y}_j y_j+O(h^2),$$

from which (13) follows.

3. Implementation of the correction procedures.

Formally, the two correction procedures (14) and (16) become

$$\tilde{\lambda}_k^{(n)} = \lambda_k^{(n)}+\mu_k^2-4\sin^2(\tilde{\mu}_k h/2)/h^2, \qquad k = 0,1,\ldots,n, \qquad n = 1,2,\ldots,$$

and

$$\tilde{\tilde{\lambda}}_k^{(n)} = \lambda_k^{(n)}+\tilde{\lambda}_k-\tilde{\lambda}_k^{(n)}, \qquad k = 0,1,\ldots,n, \qquad n = 1,2,\ldots.$$

Before they can be implemented computationally, explicit estimates are required for μ_k and $\tilde{\mu}_k$ in the former, and for $\tilde{\lambda}_k$ and $\tilde{\lambda}_k^{(n)}$ in the latter.

If approximations for μ_k and $\tilde{\mu}_k$ are derived using the iterative formulas

(26) $$\mu_k^{(j)} = k-1+f(\mu_k^{(j-1)}), \qquad \mu_k^{(0)} = k-1,$$ and

(27) $$\tilde{\mu}_k^{(j)} = k-1+f(\sin(\tilde{\mu}_k^{(j-1)}h)/h), \qquad \tilde{\mu}_k^{(0)} = k-1,$$ where

$$f(z) = \{\sin^{-1}(\alpha_2/(\alpha_2^2+\alpha_1^2z^2)^{-1/2})+\sin^{-1}(\beta_2/(\beta_2^2+\beta_1^2z^2)^{-1/2})\}/\pi,$$

then the following simple but effective correction formula is obtained

(28) $$\tilde{\lambda}_k^{(n)} = \lambda_k^{(n)}+(\mu_k^{(1)})^2-4\sin^2((\tilde{\mu}_k^{(1)})h/2)/h^2.$$

As a direct consequence of the way in which $\tilde{\lambda}_k$ was derived from $\tilde{\lambda}_k^{(n)}$ (as explained in section 2), it follows that

$$\tilde{\lambda}_k-\tilde{\lambda}_k^{(n)} = \gamma_k-\gamma_k^{(n)}+O(h^2).$$

But we already know that $\gamma_k-\gamma_k^{(n)}$ defines an $O(h^2)$ accurate correction which shows immediately that $\tilde{\lambda}_k-\tilde{\lambda}_k^{(n)}$ also yields an $O(h^2)$ accurate correction. If μ_k and $\tilde{\mu}_k$ are approximated respectively by $\mu_k^{(2)}$ and $\tilde{\mu}_k^{(2)}$, as defined by (26) and (27), and these approximations are substituted in $\tilde{\lambda}_k$ and $\tilde{\lambda}_k^{(n)}$ of (19) and (20) to yield $[\tilde{\lambda}_k]^{(2)}$ and $[\tilde{\lambda}_k^{(n)}]^{(2)}$, respectively, then we obtain the following correction formula based on (16)

(29) $$\hat{\tilde{\lambda}}_k^{(n)} = \tilde{\lambda}_k^{(n)}+[\tilde{\lambda}_k]^{(2)}-[\tilde{\lambda}_k^{(n)}]^{(2)},$$

for which it can be shown that $\hat{\tilde{\lambda}}_k^{(n)}-\lambda_k = O(h^2)$.

We verify numerically the theoretical results and estimates derived above by considering the problem

$$-y''+\exp(x)y = \lambda y, \qquad y'(0)-y(0) = y'(\pi)+y(\pi) = 0.$$

Table 1 *Comparison of corrected eigenvalues and asymptotic eigenvalues with the exact*

k	λ_k	$\lambda_k-\lambda_k^{(50)}$	$\tilde{\varepsilon}_k^{(50)}$	$\hat{\tilde{\varepsilon}}_k^{(50)}$	$\bar{\tilde{\varepsilon}}_k^{(50)}$
0	3.3346e+00	1.161e−04	1.16e−04	1.16e−04	3.33e+00
5	3.4065e+01	2.075e−01	1.70e−03	−2.04e−03	2.59e−01
10	1.0846e+02	3.251e+00	3.25e−03	−6.42e−04	1.47e−02
15	2.3338e+02	1.618e+01	4.84e−03	−2.77e−04	2.80e−03
19	3.6936e+02	4.090e+01	6.67e−03	−1.82e−04	1.07e−03

The effectiveness of the correction formulas (28) and (29) are compared in Table 1 which lists in successive columns λ_k (estimated using extrapolation applied to finite difference estimates obtained on grids of 200, 400, 800 and 1600 points); $\lambda_k-\lambda_k^{(50)}$ (the error associated with using the standard algebraic eigenvalues); $\tilde{\varepsilon}_k^{(50)} = \lambda_k-\tilde{\lambda}_k^{(50)}$; $\hat{\tilde{\varepsilon}}_k^{(50)} = \lambda_k-\hat{\tilde{\lambda}}_k^{(50)}$; and $\bar{\tilde{\varepsilon}}_k^{(50)} = \lambda_k-\tilde{\lambda}_k$ (a comparison of the asymptotic eigenvalues with the exact).

It is clear that

(i) The simple correction procedure based on $\tilde{\lambda}_k^{(50)}$ works well. For example, it estimates the error in $\lambda_{19} = \lambda_{19}^{(50)} \simeq 40.90$ correctly to two decimal places (4 significant places).

(ii) The more complex correction procedure based on $\hat{\tilde{\lambda}}_k^{(50)}$ yields a highly accurate estimate (correct to at least the third decimal place) for λ_k for $k \geqslant 9$, and thereby establishes the utility of the correction procedure for Sturm–Liouville eigenvalue problems with general boundary conditions.

(iii) Even for the relatively small k (e.g. $k \simeq 15$) the asymptotic estimate $\tilde{\lambda}_k$ yields a reliable estimate of λ_k.

The $O(h^2)$ convergence of both the estimates $\tilde{\lambda}_k^{(n)}$ and $\hat{\tilde{\lambda}}_k^{(n)}$ is illustrated in Table 2.

Table 2 *Verification of $O(h^2)$ Convergence for $\tilde{\lambda}_k^{(50)}$ and $\hat{\tilde{\lambda}}_k^{(50)}$*

k	$\tilde{\varepsilon}_k^{(50)}$	$\tilde{\varepsilon}_k^{(100)}$	$\tilde{\varepsilon}_k^{(200)}$	k	$\hat{\tilde{\varepsilon}}_k^{(50)}$	$\hat{\tilde{\varepsilon}}_k^{(100)}$	$\hat{\tilde{\varepsilon}}_k^{(200)}$
0	1.16e−04	2.91e−05	7.27e−06	0	1.16e−04	2.91e−05	7.27e−06
5	1.70e−03	3.73e−04	9.00e−05	5	−2.04e−03	−5.17e−04	−1.30e−04
10	3.25e−03	6.34e−04	1.48e−04	10	−6.42e−04	−1.61e−04	−4.03e−05
15	4.84e−03	7.69e−04	1.69e−04	15	−2.77e−04	−6.81e−05	−1.70e−05
19	6.67e−03	8.66e−04	1.78e−04	19	−1.82e−04	−4.18e−05	−1.05e−05

REFERENCES

1. R. S. Anderssen and F. R. de Hoog, *On the correction of finite difference eigenvalue approximations for Sturm-Liouville problems with general boundary conditions*, Centre for Mathematical Analysis Report CMA-R05-82, Australian National University (1982).
2. A. L. Andrew, *Computation of higher Sturm-Liouville eigenvalues*, Congressus Numerantium 34 (1982), 3–16.
3. F. R. de Hoog and R. S. Anderssen, *Asymptotic formulas for the eigenvalues and eigenfunctions of continuous and discrete eigenvalue problems in Liouville normal form* (in preparation).
4. G. Fix, *Asymptotic eigenvalues of Sturm-Liouville systems*, J. Math. Anal. Appl. 19 (1967), 519–525.
5. J. W. Paine, *Numerical Approximation of Sturm-Liouville Eigenvalues*, Ph.D. thesis, Australian National University (1979).
6. J. W. Paine and R. S. Anderssen, *Uniformly valid approximation of eigenvalues of Sturm-Liouville problems in geophysics*, Geophys. J. Roy. Astronom. Soc. 63 (1980), 441–465.
7. J. W. Paine and A. L. Andrew, *Bounds on higher-order estimates for Sturm-Liouville eigenvalues*, J. Math. Anal. Appl. 96 (1983), 388–394.
8. J. Paine and F. de Hoog, *Uniform estimation of the eigenvalues of Sturm-Liouville problems*, J. Austral. Math. Soc. (Ser. B) 21 (1980) 365–383.
9. J. W. Paine, F. R. de Hoog and R. S. Anderssen, *On the correction of finite difference eigenvalue approximation for Sturm-Liouville problems*, Computing 26 (1981), 123–139.
10. B. N. Parlett, *The Symmetric Eigenvalue Problem*, Englewood Cliffs, Prentice-Hall, N. J. (1980).
11. S. Pruess, *Estimating the eigenvalues of Sturm-Liouville problems by approximating the differential equation*, SIAM J. Numer. Anal. 10 (1973), 55–68.
12. S. Pruess, *Higher order approximations to Sturm-Liouville eigenvalues*, Numer. Math. 24 (1975), 241–247.