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# On the Correction of Finite Difference Eigenvalue Approximations for Sturm-Liouville Problems

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**Abstract — Zusammenfassung**

**On the Correction of Finite Difference Eigenvalue Approximations for Sturm-Liouville Problems.** The use of algebraic eigenvalues to approximate the eigenvalues of Sturm-Liouville operators is known to be satisfactory only when approximations to the fundamental and the first few harmonics are required. In this paper, we show how the asymptotic error associated with related but simpler Sturm-Liouville operators can be used to correct certain classes of algebraic eigenvalues to yield uniformly valid approximations.

**Zur Korrektur der Differenzen-Eigenwertapproximationen bei Sturm-Liouville-Problemen.** Die Benutzung algebraischer Eigenwerte zur näherungsweisen Berechnung der Eigenwerte von Sturm-Liouville-Operatoren ist bekanntlich nur für die Grundschwingung und einige weitere Harmonische zufriedenstellend. In dieser Arbeit zeigen wir, wie man den asymptotischen Fehler, der bei verwandten aber einfachen Sturm-Liouville-Operatoren auftritt, dazu benutzen kann, um gewisse Klassen algebraischer Eigenwerte so zu korrigieren, daß die gleichmäßig gute Approximationen liefern.

## 1. Introduction

When the coefficients involved are sufficiently smooth, the study of Sturm-Liouville eigenvalue problems, with appropriate boundary conditions, reduces to a study of the canonical Liouville normal form (cf. Paine and de Hoog [6], Section 5, where a numerical implementation of the Liouville transformation can be found)

$$-y''+q\,y=\lambda\,y,\; q=q\,(x),\; y=y\,(x),\; y''=d^2\,y/d\,x^2,\; 0\leq x\leq\pi, \tag{1.1}$$

$$y\,(0)=y\,(\pi)=0. \tag{1.2}$$

In this paper, we examine numerical techniques for the approximate determination of the eigenvalues of (1.1)—(1.2).

If, on a grid

$$\boldsymbol{G}=\{x_j;\, x_j=j\,h, j=0, 1, 2, \ldots, n+1,\, h=\pi/(n+1)\}, \tag{1.3}$$

finite difference approximations are used to replace (1.1)—(1.2) by an algebraic eigenvalue problem of order $n$ (viz.



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$$(-A+D)\underline{u}=\lambda^{(n)}\underline{u}, \tag{1.4}$$

where $D\equiv 0$ if and only if $q\equiv 0$), then it is well known that the algebraic eigenvalues $\lambda_1^{(n)}, \lambda_2^{(n)}, \ldots, \lambda_n^{(n)}$ of (1.4) only yield satisfactory approximations for the fundamental $\lambda_1$ and the first few harmonics $\lambda_2, \lambda_3, \ldots, \lambda_m\,(m\ll n)$. For example, if $q\equiv 0$ and a central difference formula is used to approximate $-y''$ on $G$, then the corresponding algebraic eigenvalues (i.e. the eigenvalues of $-A$) are given by

$$4\sin^2(k\,h/2)/h^2,\ k=1,2,\ldots,n,$$

while the corresponding error is

$$\varepsilon_k^{(n)}=k^2-4\sin^2(k\,h/2)/h^2,\ k=1,2,\ldots,n, \tag{1.5}$$

which satisfies

$$\varepsilon_k^{(n)}=O(k^4\,h^2).$$

This clearly illustrates the rapid growth of $\varepsilon_k^{(n)}$ as a function of $k$.

Numerical techniques which avoid this difficulty and thereby guarantee uniformly valid approximate eigenvalues have been proposed by Paine and de Hoog [6] (cf. Pruess [7]). They construct the approximate eigenvalues as the exact eigenvalues of a differential eigenvalue problem which is a suitably close approximation to (1.1)—(1.2). In addition, Paine [5] has shown that, when Heun's method is used to integrate the modified Prüfer phase for (1.1)—(1.2), uniformly valid approximate eigenvalues are generated.

In this paper, we show how approximate algebraic eigenvalues $\lambda_k^{(n)}$ derived for (1.1)—(1.2) for general $q$ can be corrected to yield substantially improved approximations. The idea is basically simple. Because the eigenvalues of

$$-y''=\mu\,y,\ y(0)=y(\pi)=0,$$

are known (viz. $\mu_k=k^2$), and the algebraic eigenvalues defined by

$$-A\,\underline{u}=\mu^{(n)}\,\underline{u}$$

can often be evaluated analytically, the error

$$k^2-\mu_k^{(n)}$$

can be used to estimate the asymptotic behaviour of $\lambda_k-\lambda_k^{(n)}$, and thereby generate the corrected eigenvalue approximations

$$\tilde{\lambda}_k^{(n)}=\lambda_k^{(n)}+k^2-\mu_k^{(n)}.$$

In the sequel, we limit attention to the situation where central differences have been used to approximate $-y''+q\,y$ on $G$. Then

$$k^2-\mu_k^{(n)}=\varepsilon_k^{(n)}.$$

where $\varepsilon_k^{(n)}$ is given by (1.5), and the corresponding corrected eigenvalues are given by

$$\tilde{\lambda}_k^{(n)}=\lambda_k^{(n)}+\varepsilon_k^{(n)}.$$

We prove that, when $q\in C^2[0,\pi]$, there exists an $\alpha$, independent of $n$, such that

$$\lambda_k^{(n)}+\varepsilon_k^{(n)}=\lambda_k+O(k\,h^2),\ 1\le k\le\alpha\,n,\ \alpha<1. \tag{1.6}$$

Although we do not extend this result to the more general canonical Liouville normal form

$$-y''+q\,y=\lambda\,y,\; q=q(x),\; y=y(x),\; 0<x<\pi, \tag{1.7}$$

$$\sigma_1\,y(0)+\sigma_2\,y'(0)=\theta_1\,y(\pi)+\theta_2\,y'(\pi)=0, \tag{1.8}$$

the extension of this technique to such Sturm-Liouville problems and other discretizations is discussed briefly in Section 5.

## 2. Notation and Preliminaries

For the eigenvalue problem (1.1)—(1.2), we derive a number of basic properties about its $k$-th eigenvalue $\lambda_k$ and corresponding eigenfunction $y(x)$.

Let $\boldsymbol{G}$ denote the grid (1.3) and introduce the notation

$$\underset{\sim}{f}=(f(x_1),\ldots,f(x_n))^T$$

for functions $f$ defined on $[0,\pi]$. In addition, we shall use the notation

$$s(x)=\sin kx.$$

Using the standard central difference formula to approximate $-y''$ on $\boldsymbol{G}$, the eigenvalue problem (1.1)—(1.2) is replaced by the algebraic problem

$$(-A+D)\,\underset{\sim}{u}=\lambda^{(n)}\,\underset{\sim}{u} \tag{2.1}$$

with

$$D=\operatorname{diag}(q(x_1),\ldots,q(x_n)),$$

and

$$A=\frac{1}{h^2}\cdot\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \cdot & \cdot & \cdot & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix}. \tag{2.2}$$

We denote the $k$-th eigenvalue and eigenvector of (2.1) by $\lambda_k^{(n)}$ and $\underset{\sim}{u}=(u_1,\ldots,u_n)^T$. When $D\equiv 0$, it is easy to verify that

$$4\sin^2(k\,h/2)/h^2,\quad k=1,2,\ldots,n, \tag{2.3}$$

and $\underset{\sim}{s}$ define the $k$-th eigenvalue and eigenvector of $-A$, respectively; i.e.

$$-A\,\underset{\sim}{s}=\frac{4\sin^2(k\,h/2)}{h^2}\,\underset{\sim}{s},\quad k=1,2,\ldots,n. \tag{2.4}$$

We initially derive a number of results about the asymptotic behaviour of $\lambda_k$ and $y(x)$ of (1.1)—(1.2), which will be required subsequently.

It is well known (cf. Fix [2], Corollary 3) that

$$\lambda_k=k^2+\frac{1}{\pi}\int_0^{\pi} q(t)\,dt+O(k^{-2}). \tag{2.5}$$

Without loss of generality, we assume that

$$\int_0^\pi q(t)\,dt=0,$$

since it imposes the same constant translation on each of the $\lambda_k$ and $\lambda_k^{(n)}$. Under this assumption, it follows that

$$\lambda_k=k^2+O(k^{-2}). \tag{2.6}$$

Next, we derive a general result about the behaviour of $y(x)$ in terms of the eigenvalues and eigenfunctions of (1.1)—(1.2) when $q(x)\equiv 0$.

**Lemma 2.1:** *The general eigenfunction of* (1.1)—(1.2) *satisfies*

$$y(x)=\sin kx+e(x), \tag{2.7}$$

*with*

$$e(x)=\frac{1}{k}w(x)+\frac{1}{k^2}v(x)+\frac{1}{k^3}z(x) \tag{2.8}$$

*where*

$$w(x)=\int_0^x q(\tau)\sin k\tau\sin k(x-\tau)\,d\tau, \tag{2.9}$$

*and*

$$v(x)=\int_0^x w(\tau)\sin k\tau\sin k(x-\tau)\,d\tau. \tag{2.10}$$

*In addition,*

$$w^{(l)}(x)=O(k^l),\ v^{(l)}(x)=O(k^l),\ z^{(l)}(x)=O(k^l),$$

$$e^{(l)}(x)=O(k^{l-1}),\ e(0)=e(\pi)=e^{(2)}(0)=e^{(2)}(\pi)=0,\ l=0,1,2,3,4,$$

*where the superscript denotes l-th order differentiation w.r.t. x.*

*Proof*: It is well known that a particular solution of

$$y''+\beta y=f,\ f=f(x),$$

is given by (cf. Courant and Hilbert [1], Chapter V, Section 11, eqn. (10), p. 283)

$$\frac{1}{\sqrt{\beta}}\int_0^x f(\tau)\sin\sqrt{\beta}(x-\tau)\,d\tau.$$

Thus, the most general solution satisfying $y(0)=0$ is

$$y(x)=C_1\sin\sqrt{\beta}\,x+\frac{1}{\sqrt{\beta}}\int_0^x f(\tau)\sin\sqrt{\beta}(x-\tau)\,d\tau. \tag{2.11}$$

Now, consider the eigenvalue problem

$$-y''+q(x)y=\lambda_k y,\ y(0)=y(\pi)=0,$$

which can be rewritten as

$$y''+k^2y=(k^2-\lambda_k+q(x))\,y,\ y(0)=y(\pi)=0. \tag{2.12}$$

From (2.11), it follows that

$$y(x)=C_1 \sin k x+\frac{1}{k}\int_0^x (k^2-\lambda_k+q(\tau))\sin k(x-\tau)\, y(\tau)\, d\tau.$$

Since the eigenfunction $y$ is arbitrary up to a scalar multiple, we set $C_1=1$. Applying the Picard iteration method (i.e. the method of successive substitutions) to this equation with $\sin k x$ as the initial iterate and recalling from (2.6) that $k^2-\lambda_k=O(k^{-2})$, we obtain the required (2.7) and (2.8). ∎

We now turn to the construction of a discrete analogue of (2.7) on $\boldsymbol{G}$.

For an explicit characterization of the behaviour of $\lambda_k^{(n)}$ and $\underline{u}$ in terms of $\mu_k^{(n)}$, $q$, etc., we require the following two Lemmas.

**Lemma 2.2:** *For $\beta \neq p\pi$, $p=0, 1, \ldots$,*

$$\exp(-i\beta l)\sum_{r=0}^{l}\exp(2i\beta r)=\sin((l+1)\beta)/\sin\beta. \tag{2.13}$$

*Proof*: Follows immediately from standard trigonometric manipulations. ∎

**Lemma 2.3:** *For $\beta \neq r\pi$, $r=0, 1, 2, \ldots$, a particular solution of the difference equation*

$$u_{p+1}-2\cos\beta\, u_p+u_{p-1}=d_p, \quad p=1, 2, \ldots, n, \tag{2.14}$$

*is given by*

$$u_p=\left\{\sum_{j=1}^{p}\sin(\beta(p-j))\, d_j\right\}/\sin\beta. \tag{2.15}$$

*Proof*: Writing

$$z_p=u_p-b\, u_{p-1}, \quad u_0=u_1=0, \tag{2.16}$$

with $a b=1$ and $a+b=2\cos\beta$, (2.14) becomes

$$z_{p+1}-a z_p=d_p.$$

As an immediate consequence, it follows that

$$z_{p+1}=\sum_{j=1}^{p} a^{p-j} d_j,$$

and hence, from (2.16)

$$u_{p+1}=\sum_{j=1}^{p} b^{p-j}\sum_{r=1}^{j} a^{j-r} d_r. \tag{2.17}$$

Using summation by parts, (2.17) becomes

$$\begin{aligned} u_{p+1} &=\sum_{j=1}^{p} d_j \sum_{r=j}^{p} a^{r-j} b^{p-r} \\ &=\sum_{j=1}^{p} d_j \sum_{r=0}^{p-j} a^{r} b^{p-r-j} \\ &=\sum_{j=1}^{p} d_j \left\{b^{p-j}\sum_{r=0}^{p-j} a^{r} b^{-r}\right\}. \end{aligned}$$

Since $a=\exp(i\beta)$ and $b=\exp(-i\beta)$, it now follows from Lemma 2.2 that

$$u_{p+1}=\sum_{j=1}^{p} d_j \sin(\beta(p+1-j))/\sin\beta. \qquad \blacksquare$$

We are now in a position to prove

**Theorem 2.1:** *For $k\leq n$ and $q(x_j)=O(1), j=0,1,2,\ldots,n+1$,*

$$|\lambda_k^{(n)}-\mu_k^{(n)}|=O(1),\quad k=1,2,\ldots,n, \tag{2.18}$$

*and the corresponding eigenfunction $\underset{\sim}{u}$ satisfies*

$$u_j=\sin k x_j+\frac{h^2}{\sin hk}\sum_{l=1}^{j} \sin k(x_j-x_l)\{\mu_k^{(n)}-\lambda_k^{(n)}+q_l\} u_l. \tag{2.19}$$

*Proof*: The result (2.18) is an immediate consequence of perturbation theory for the eigenvalues of symmetric matrices (cf. Wilkinson [8], Chapter 2, Section 44, p. 101).

To prove (2.19), we first observe from (2.1) that

$$u_{p+1}-2u_p+u_{p-1}=h^2(-\lambda_k^{(n)}+q_p)u_p,$$

and hence, on adding $h^2\mu_k^{(n)}u_p$ to both sides of this equation,

$$u_{p+1}-2\cos(kh)u_p+u_{p-1}=h^2\{\mu_k^{(n)}-\lambda_k^{(n)}+q_p\}u_p. \tag{2.20}$$

Since the boundary conditions (1.2) imply that $u_0=0$, it follows that the homogeneous solution associated with the left hand side of (2.20) is $C_1 \sin k x_j$. As in Lemma 2.1, we may set $C_1\equiv 1$. Hence, on applying Lemma 2.3 to (2.20), we obtain (2.19) as its general solution. ■

**Corollary 2.1:** *If $kh\leq\alpha\pi$, $\alpha<1$, then*

$$u_j=\sin k x_j+\beta_j,$$

*with $\beta_j=O(1/k)$.*

*Proof*: This is an immediate consequence of (2.18), the assumption that $q(x_j)=O(1)$, $j=0,1,2,\ldots,n+1$, and the facts that the number of terms in the summation in (2.19) is bounded by $O(1/h)$ and

$$kh/\sin kh=O(1). \qquad \blacksquare$$

## 3. Error Estimates for $\lambda_k^{(n)}$

In order to derive the error estimate (1.5)—(1.6), it is necessary to examine in some detail the asymptotic behaviour of $\lambda_k-\lambda_k^{(n)}$. Since

$$-\underset{\sim}{y}''+D\underset{\sim}{y}=\lambda_k\underset{\sim}{y}$$

and

$$-A\underset{\sim}{u}+D\underset{\sim}{u}=\lambda_k^{(n)}\underset{\sim}{u},$$

it follows that

$$\lambda_k-\lambda_k^{(n)}=\{\underset{\sim}{u}^T A\underset{\sim}{y}-\underset{\sim}{u}^T\underset{\sim}{y}''\}/\underset{\sim}{u}^T\underset{\sim}{y}$$

provided that $\underset{\sim}{u}$ is not orthogonal to $\underset{\sim}{y}$.

Since, from (2.7), $\underset{\sim}{y}=\underset{\sim}{s}+\underset{\sim}{e}$, it follows that

$$\underset{\sim}{u}^T A \underset{\sim}{y}-\underset{\sim}{u}^T \underset{\sim}{y}''=\varepsilon_k^{(n)} \underset{\sim}{u}^T \underset{\sim}{s}+\underset{\sim}{u}^T (A \underset{\sim}{e}-\underset{\sim}{e}'') \tag{3.1}$$

after using (2.3), (2.4) and the definition of $\underset{\sim}{s}$ and $\varepsilon_k^{(n)}$. If the result of Corollary 2.1 (i.e. $\underset{\sim}{u}=\underset{\sim}{s}+\beta$ with $\beta_j=O(1/k)$) is applied to (3.1), we obtain

$$\underset{\sim}{u}^T A \underset{\sim}{y}-\underset{\sim}{u}^T \underset{\sim}{y}''=\varepsilon_k^{(n)} \underset{\sim}{u}^T \underset{\sim}{s}+\underset{\sim}{s}^T (A \underset{\sim}{e}-\underset{\sim}{e}'')+\underset{\sim}{\beta}^T (A \underset{\sim}{e}-\underset{\sim}{e}''). \tag{3.2}$$

We now derive estimates for the last two terms on the right hand side of (3.2). We consider the third term first.

**Lemma 3.1:**

$$\frac{w_{j+1}-2 w_j+w_{j-1}}{h^2}=\varepsilon_k^{(n)} w_j+w_j''+O(k^3 h^2). \tag{3.3}$$

*Proof*: Let

$$\eta(x,h)=\int_x^{x+h} q(\tau)\sin k\tau \sin k(x+h-\tau)\,d\tau$$

$$=h\int_0^1 q(x+\tau h)\sin k(x+\tau h)\sin\big(k h(1-\tau)\big)\,d\tau.$$

Clearly, using the notation $\eta^{(p)}(x,h)=\partial^p \eta(x,h)/\partial h^p$,

$$\eta(x,0)=0,\ \eta^{(1)}(x,0)=0,\ \eta^{(2)}(x,0)=k q(x)\sin k x$$

and

$$\eta^{(p)}(x,0)=O(k^{p-1}).$$

It therefore follows that

$$\begin{aligned}\frac{\eta(x_j,h)-2\eta(x_j,0)+\eta(x_j,-h)}{h^2}&=\eta^{(2)}(x_j,0)+O(k^3 h^2)\\&=k q(x_j)\sin k x_j+O(k^3 h^2).\end{aligned} \tag{3.4}$$

From (2.9), it follows that

$$w(x_j+h)=\int_0^{x_j} q(\tau)\sin k\tau \sin k(x_j+h-\tau)\,d\tau+\eta(x_j,h)$$

and consequently that

$$\begin{aligned}\frac{w_{j+1}-2w_j+w_{j-1}}{h^2}&=\frac{1}{h^2}\int_0^{x_j} q(\tau)\sin k\tau\,\{\sin k(x_j+h-\tau)-2\sin k(x_j-\tau)\\&\qquad+\sin k(x_j-h-\tau)\}\,d\tau\\&\quad+\big(\eta(x_j,h)-2\eta(x_j,0)+\eta(x_j,-h)\big)/h^2\\&=-\frac{4\sin^2(k h/2)}{h^2}\,w(x_j)+k q(x_j)\sin k x_j+O(k^3 h^2)\end{aligned}$$

on using (3.4) and appropriate trigonometric relationships. Incorporating the fact that

$$k q(x)\sin k x=w''(x)-k^2 w(x)$$

into this last expression along with the definition (2.3) of $\mu_k^{(n)}$, we obtain the required (3.3). ■

**Lemma 3.2:**

$$(A\,\underset{\sim}{e})_j=\varepsilon_k^{(n)}\,e_j+e_j''+O\,(k^2\,h^2). \tag{3.5}$$

*Proof*: It follows from (2.8) that

$$e\,(x)=\frac{1}{k}\,w\,(x)+\frac{1}{k^2}\,g\,(x),$$

where $g\,(x)=v\,(x)+\frac{1}{k}\,z\,(x)$, and hence, because $e_0=e_{n+1}=0$,

$$\begin{aligned}(A\,e)_j&=\frac{e_{j-1}-2\,e_j+e_{j+1}}{h^2},\quad j=1,\ldots,n\\ &=\frac{1}{k}\left(\frac{w_{j-1}-2\,w_j+w_{j+1}}{h^2}\right)+\frac{1}{k^2}\left(\frac{g_{j-1}-2\,g_j+g_{j+1}}{h^2}\right)\\ &=\frac{1}{k}\left(\frac{w_{j-1}-2\,w_j+w_{j+1}}{h^2}\right)+\frac{1}{k^2}\,g_j''+O\,(k^2\,h^2)\end{aligned}$$

on interpreting $(g_{j-1}-2\,g_j+g_{j+1})/h^2$ as a central difference approximation to $g''$ on $\boldsymbol{G}$ at $x_j$. Using Lemma 3.1, this last equation becomes

$$(A\,\underset{\sim}{e})_j=\frac{1}{k}\,\varepsilon_k^{(n)}\,w_j+\frac{1}{k}\,w_j''+\frac{1}{k^2}\,g_j''+O\,(k^2\,h^2),$$

and hence the required result (3.5) is obtained on using the fact that

$$\frac{1}{k^2}\,\varepsilon_k^{(n)}\,g_j=O\,(k^2\,h^2).$$ ■

As a direct consequence of this lemma, we obtain the required estimate for the third term on the right hand side of (3.2):

**Corollary 3.1:**

$$\underset{\sim}{\beta}^T\,(A\,\underset{\sim}{e}-\underset{\sim}{e}'')=\varepsilon_k^{(n)}\,\underset{\sim}{\beta}^T\,\underset{\sim}{e}+O\,(k\,h). \tag{3.6}$$

*Proof*: It is only necessary to recall that $\beta_j=O\,(1/k)$. ■

Because the components of $\underset{\sim}{s}$ are order 1, the estimate (3.5) cannot be used to show that

$$\underset{\sim}{s}^T\,(A\,\underset{\sim}{e}-\underset{\sim}{e}'')=\varepsilon_k^{(n)}\,\underset{\sim}{s}^T\,\underset{\sim}{e}+O\,(k\,h).$$

It is necessary to exploit the specific properties of $\underset{\sim}{s}$ and $\underset{\sim}{e}$ before such a sharp estimate can be obtained. Initially, we observe that

$$\underset{\sim}{s}^T\,(A\,\underset{\sim}{e}-\underset{\sim}{e}'')=\varepsilon_k^{(n)}\,\underset{\sim}{s}^T\,\underset{\sim}{e}-\underset{\sim}{s}^T\,(\underset{\sim}{e}''+k^2\,\underset{\sim}{e}). \tag{3.7}$$

The required result then follows from (3.7) the moment we prove

**Lemma 3.3:** *Under the assumption that $q''\,(x)$ is continuous on $[0,\pi]$,*

$$\underset{\sim}{s}^T\,(\underset{\sim}{e}''+k^2\,\underset{\sim}{e})=O\left(k\,h+(n-k)^{-2}\,h^{-1}\right). \tag{3.8}$$

For the proof of this lemma, we shall make repeated use of the error formula for the trapezoidal rule and therefore state it as a lemma (cf. Isaacson and Keller [3], p. 316).

**Lemma 3.4:** *Let $f$ denote any function with a continuous second derivative on the interval $[0, \pi]$, and consider the use of the trapezoidal rule on the grid $\boldsymbol{G}$ viz.*

$$h \sum_{j=0}^{n+1}{}' f(x_j) = h \left\{\frac{1}{2} f(x_0) + f(x_1) + \ldots + \frac{1}{2} f(x_{n+1})\right\},$$

*for the approximate integration of* $\int_0^\pi f(x)\,dx$. *Then*

$$h \sum_{j=0}^{n+1}{}' f(x_j) = \int_0^\pi f(x)\,dx + \frac{h^2}{12} f^{(2)}(\xi), \quad \xi \in (0, \pi). \tag{3.9}$$

We now use (3.9) to establish the following estimates

**Lemma 3.5:** *Under the assumption that $q''(x)$ is continuous on $[0, \pi]$,*

$$\frac{1}{k^3} \sum_{j=0}^{n+1}{}' s_j (z_j'' + k^2 z_j) = \frac{1}{h k^3} \int_0^\pi \sin k\tau \left(z''(\tau) + k^2 z(\tau)\right) d\tau + O(k h); \tag{3.10}$$

$$\frac{1}{k^2} \sum_{j=0}^{n+1}{}' s_j (v_j'' + k^2 v_j) = \frac{1}{h k^2} \int_0^\pi \sin k\tau \left(v''(\tau) + k^2 v(\tau)\right) d\tau + O(h k); \tag{3.11}$$

$$\begin{aligned} \frac{1}{k} \sum_{j=0}^{n+1}{}' s_j (w_j'' + k^2 w_j) = {} & \frac{1}{h k} \int_0^\pi \sin k\tau \left(w''(\tau) + k^2 w(\tau)\right) d\tau \\ & - \frac{1}{2h} \int_0^\pi q(\tau) \cos\left(2(n+1-k)\tau\right) d\tau + O(h). \end{aligned} \tag{3.12}$$

*Proof*: The estimate (3.10) is an immediate consequence of the application of (3.9) to $f(x) = \sin kx\,(z'' + k^2 z)$ on using the result of Lemma 2.1 that $z^{(l)}(x) = O(k^l)$, $l = 0, 1, 2, \ldots, 4$. Once it is observed that

$$f(x) = \sin kx\,(v'' + k^2 v) = k \sin kx\, q(x)\, w(x),$$

the estimate (3.11) follows using a similar argument.

For (3.12), we use the fact that

$$w'' + k^2 w = k \sin kx\, q(x)$$

and obtain

$$\frac{1}{k} \sum_{j=0}^{n+1}{}' s_j (w_j'' + k^2 w_j) = \frac{1}{2} \sum_{j=0}^{n+1}{}' q(x_j) - \frac{1}{2} \sum_{j=0}^{n+1}{}' q(x_j) \cos(2 k x_j). \tag{3.13}$$

Using the fact that, by assumption, $\int_0^\pi q(\tau)\,d\tau = 0$, we obtain, on applying (3.9) to the first term on the right hand side of (3.13),

$$\sum_{j=0}^{n+1}{}' q(x_j) = O(h). \tag{3.14}$$

For the second term, we use the Fourier cosine expansion for $q(t)$; viz.

$$q(x)=\sum_{r=0}^{\infty} q_r \cos r x, \tag{3.15}$$

with

$$q_r=\frac{2}{\pi}\int_0^{\pi} q(x)\cos r x\, dx. \tag{3.16}$$

Because of the assumption that $q''(x)$ is continuous on $[0, \pi]$, integration by parts can be applied to (3.16) to show that

$$q_r=O(r^{-2}),\ r=1, 2, \ldots. \tag{3.17}$$

Substitution of (3.13) into the second term yields

$$\begin{aligned}\sum_{j=0}^{n+1}{}' q(x_j)\cos k x_j &= \sum_{r=0}^{\infty} q_r \sum_{j=0}^{n+1}{}' \cos r x_j \cos 2 k x_j\\ &=\frac{1}{2}\sum_{r=0}^{\infty} q_r \sum_{j=0}^{n+1}{}' \{\cos(r+2k)x_j+\cos(r-2k)x_j\}.\end{aligned} \tag{3.18}$$

Since

$$\sum_{j=0}^{n+1}{}' \cos\left(\frac{\beta j \pi}{n+1}\right)=\begin{cases} n+1, & \beta=0,\ 2(n+1),\ 4(n+1), \ldots,\\ 0, & \beta=\text{integer},\ \beta\neq 0, 2(n+1), \ldots,\end{cases}$$

it follows that

$$\begin{aligned}\sum_{j=0}^{n+1}{}' q(x_j)\cos 2 k x_j &=\frac{n+1}{2}\{q_{2(n+1)-k}+q_{4(n+1)-2k}+\ldots\}\\ &+\frac{n+1}{2}\{q_{2k}+q_{2(n+1)+2k}+\ldots\}\end{aligned}$$

and hence, on invoking (3.16) and (3.17),

$$\begin{aligned}\sum_{j=0}^{n+1}{}' q(x_j)\cos 2 k x_j &=\frac{1}{h}\left\{\int_0^{\pi} q(\tau)\cos 2 k \tau\, d\tau+\right.\\ &\left.+\int_0^{\pi} q(\tau)\cos(2(n+1-k)\tau)\, d\tau\right\}+O(h).\end{aligned}$$

Substitution of this result back into (3.13) along with (3.14) yields

$$\begin{aligned}\frac{1}{k}\sum_{j=0}^{n+1}{}' s_j(w_j''+k^2 w_j) &= -\frac{1}{2h}\int_0^{\pi} q(\tau)\cos 2 k \tau\, d\tau\\ &-\frac{1}{2h}\int_0^{\pi} q(\tau)\cos(2(n+1-k)\tau)\, d\tau+O(h).\end{aligned}$$

The required result (3.12) now follows on using the fact that

$$-\frac{1}{2}\int_0^{\pi} q(\tau)\cos 2 k \tau\, d\tau=\frac{1}{k}\int_0^{\pi}(w''(\tau)+k^2 w(\tau))\sin k \tau\, d\tau.$$ ■

We are now in a position to prove Lemma 3.3.

*Proof of Lemma 3.3*: Initially, we observe that

$$\underset{\sim}{s}^T(\underset{\sim}{e}''+k^2\underset{\sim}{e})=\frac{1}{k}\sum_{j=0}^{n+1}{}' s_j(w_j''+k^2 w_j)$$
$$+\frac{1}{k^2}\sum_{j=0}^{n+1}{}' s_j(v_j''+k^2 v_j)+\frac{1}{k^3}\sum_{j=0}^{n+1}{}' s_j(z_j''+k^2 z_j).$$

Applying (3.12), (3.11) and (3.10) to the first, second and third terms in this last expression, respectively, yields

$$\underset{\sim}{s}^T(\underset{\sim}{e}''+k^2\underset{\sim}{e})=\frac{1}{h}\int_0^\pi \sin k\tau\,(e''(\tau)+k^2 e(\tau))\,d\tau$$
$$-\frac{1}{2h}\int_0^\pi q(\tau)\cos(2(n+1-k)\tau)\,d\tau+O(kh).$$

Using the fact (from Lemma 2.1) that $e(0)=e(\pi)=e''(0)=e''(\pi)=0$, integration by parts shows that the first term on the right hand side of this last expression is zero. On the other hand, it follows from (3.17) that the second term is $O(h^{-1}(n+1-k)^{-2})$ which proves Lemma 3.3. ■

As an immediate consequence of (3.7) and Lemma 3.3, we obtain

**Lemma 3.6:** *Under the assumption that $q''(x)$ is continuous on $[0,\pi]$*

$$\underset{\sim}{s}^T(A\underset{\sim}{e}-\underset{\sim}{e}'')=\varepsilon_k^{(n)}\underset{\sim}{s}^T\underset{\sim}{e}+O(kh), \tag{3.19}$$

*for $kh\le\alpha\pi$, $\alpha<1$.*

We are now in a position to use the estimates (3.6) and (3.19) to establish our main result:

**Theorem 3.1:** *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*

$$\lambda_k-\lambda_k^{(n)}=\varepsilon_k^{(n)}+O(kh^2),\quad k\le\alpha n. \tag{3.20}$$

*Proof*: Substitution of (3.6) and (3.19) into (3.2) yields

$$\begin{aligned}(\lambda_k-\lambda_k^{(n)})\underset{\sim}{u}^T\underset{\sim}{y}=\underset{\sim}{u}^T A\underset{\sim}{y}-\underset{\sim}{u}^T\underset{\sim}{y}''&=\varepsilon_k^{(n)}\underset{\sim}{u}^T\underset{\sim}{s}+\varepsilon_k^{(n)}\underset{\sim}{s}^T\underset{\sim}{e}+\varepsilon_k^{(n)}\underset{\sim}{\beta}^T\underset{\sim}{e}+O(kh)\\&=\varepsilon_k^{(n)}\underset{\sim}{u}^T\underset{\sim}{y}+O(kh).\end{aligned} \tag{3.21}$$

In addition, it follows from Corollary 2.1 and Lemma 2.1 that

$$\underset{\sim}{u}^T\underset{\sim}{y}=\left(\frac{n}{2}\right)+O\left(\frac{n}{k}\right)=\frac{n}{2}\left(1+O\left(\frac{1}{k}\right)\right).$$

Hence, there exists a $k_0>1$, independent of $n$, such that

$$\underset{\sim}{u}^T\underset{\sim}{y}\ge Kn,\quad K=\text{const.},\quad k\ge k_0.$$

Combining this last result with (3.21) yields the required relationship (3.18) for $k_0\le k\le\alpha n$.

The situation when $k<k_0$ does not pose a problem. From Keller [4], Section 5.3, p. 135, we have

$$|\lambda_k-\lambda_k^{(n)}|\leq C h^2, \quad k<k_0,$$

which, in conjunction with (3.20) for $k_0\leq k\leq \alpha n$, guarantees a uniform error of $O(k h)$ for the corrected eigenvalue

$$\tilde{\lambda}_k^{(n)}=\lambda_k^{(n)}+\varepsilon_k^{(n)}, \quad k\leq \alpha n, \alpha<1,$$

since $\varepsilon_k^{(n)}=O(h^2)$ for $k<k_0$. ∎

## 4. Numerical Exemplification

For convenience, we introduce the notation $\tilde{\lambda}_k^{(n)}=\lambda_k^{(n)}+\varepsilon_k^{(n)}$.

The errors in the standard and corrected eigenvalue estimates for the first ten eigenvalues of

$$-y''+\exp(x)\,y=\lambda y, \quad y=y(x), \tag{4.1}$$

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

obtained using central differences to approximate $-y''$ and $n=39$, are given in Table 1. It is clear from these results that the corrected estimates are greatly superior to the original ones. In fact the estimates are so good that the structure of the error cannot be seen due to the effects of rounding error.

Table 1. *Error in the standard and corrected finite difference eigenvalue estimates for* (4.1)—(4.2)

| $k$ | $\lambda_k$ | $\lambda_k-\lambda_k^{(n)}$ | $\lambda_k-\tilde{\lambda}_k^{(n)}$ |
|---|---|---|---|
| 1 | 11.5424 | .0057 | .0006 |
| 2 | 41.1867 | .0813 | .0002 |
| 3 | 90.5404 | .4106 | .0004 |
| 4 | 159.6296 | 1.2954 | .0007 |
| 5 | 248.4569 | 3.1544 | −.0002 |
| 6 | 357.0230 | 6.5261 | −.0006 |
| 7 | 485.3281 | 12.0593 | .0001 |
| 8 | 633.3724 | 20.5083 | −.0007 |
| 9 | 801.1558 | 32.7373 | .0002 |
| 10 | 988.6783 | 49.7023 | .0001 |

A clearer illustration of the behaviour of the eigenvalue error can be obtained if instead we consider the eigenvalue problem

$$-y''+\exp(x)\,y=\lambda y, \quad y=y(x), \tag{4.3}$$

$$y(0)=y(\pi)=0. \tag{4.4}$$

The errors in the standard and corrected eigenvalue estimates using $n=39$ are given in Table 2. For the standard estimate, the error is obviously in close agreement with predicted $k^4$ growth. Also the growth in the error for the corrected estimates, displayed in Fig. 1, appears to be consistent with that predicted by Theorem 3.1.

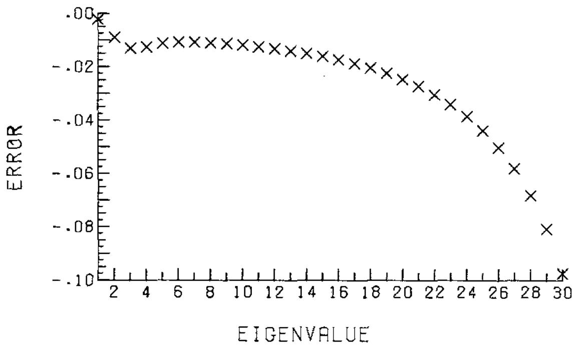


Fig. 1. The error $(\tilde{\lambda}_k^{(n)}-\lambda_k)$ associated with (4.3)—(4.4)

Table 2. *Error in the standard and corrected finite difference eigenvalue estimates for* (4.3)—(4.4)

| $k$ | $\lambda_k$ | $(\lambda_k-\lambda_k^{(n)})$ | $(\lambda_k-\lambda_k^{(n)})/k^4$ | $(\lambda_k-\tilde{\lambda}_k^{(n)})$ | $(\lambda_k-\tilde{\lambda}_k^{(n)})/k$ |
|---|---|---|---|---|---|
| 1 | 4.89667 | .0029 | .0029 | .0024 | .0024 |
| 2 | 10.04519 | .0172 | .0011 | .0091 | .0045 |
| 3 | 16.01927 | .0546 | .0007 | .0131 | .0043 |
| 4 | 23.26627 | .1437 | .0006 | .0124 | .0031 |
| 5 | 32.26371 | .3308 | .0005 | .0113 | .0023 |
| 6 | 43.22002 | .6720 | .0005 | .0107 | .0018 |
| 7 | 56.18159 | 1.2326 | .0005 | .0107 | .0015 |
| 8 | 71.15300 | 2.0889 | .0005 | .0110 | .0014 |
| 9 | 88.13212 | 3.3283 | .0005 | .0113 | .0013 |
| 10 | 107.11668 | 5.0477 | .0005 | .0118 | .0012 |
| 11 | 128.10502 | 7.3538 | .0005 | .0124 | .0011 |
| 12 | 151.09604 | 10.3617 | .0005 | .0132 | .0011 |
| 13 | 176.08900 | 14.1947 | .0005 | .0140 | .0011 |
| 14 | 203.08337 | 18.9835 | .0005 | .0150 | .0011 |
| 15 | 232.07881 | 24.8648 | .0005 | .0160 | .0011 |
| 16 | 263.07507 | 31.9814 | .0005 | .0173 | .0011 |
| 17 | 296.07196 | 40.4804 | .0005 | .0190 | .0011 |
| 18 | 331.06934 | 50.5130 | .0005 | .0204 | .0011 |
| 19 | 368.06713 | 62.2331 | .0005 | .0224 | .0012 |
| 20 | 407.06524 | 75.7968 | .0005 | .0245 | .0012 |

To further investigate the behaviour of the error in the corrected eigenvalue estimates, the eigenvalue errors for the first twenty eigenvalues of (4.3)—(4.4) for a sequence of values of $n$ are given in Table 3. If we consider the errors for a fixed value of $k$ then it is clear that the predicted second order convergence is obtained as $h\to 0$.

Table 3. *Eigenvalue errors for the corrected finite difference eigenvalue estimates for* (4.3)—(4.4)

| $k$ | $\lambda_k$ | $\lambda_k - \tilde{\lambda}_k^{(n)}$ | | |
|---|---|---|---|---|
| | | $n=19$ | $n=39$ | $n=79$ |
| 1 | 4.8967 | .0095 | .0024 | .0006 |
| 2 | 10.0452 | .0365 | .0091 | .0023 |
| 3 | 16.0193 | .0539 | .0131 | .0033 |
| 4 | 23.2663 | .0539 | .0124 | .0031 |
| 5 | 32.2637 | .0520 | .0113 | .0026 |
| 6 | 43.2200 | .0540 | .0107 | .0026 |
| 7 | 56.1816 | .0595 | .0107 | .0024 |
| 8 | 71.1530 | .0677 | .0110 | .0023 |
| 9 | 88.1321 | .0790 | .0113 | .0024 |
| 10 | 107.1167 | .0944 | .0118 | .0027 |
| 11 | 128.1050 | .1152 | .0124 | .0024 |

To illustrate that the above technique for correcting algebraic eigenvalues does in fact have general applicability, we list in Table 4 for a sequence of values of $n$ the error in the corrected eigenvalues for the following almost singular problem

$$-y'' + (x+0.1)^{-2}\, y = \lambda\, y, \quad y = y(x), \tag{4.5}$$

$$y(0) = y(\pi) = 0. \tag{4.6}$$

Table 4. *Error in the corrected finite difference eigenvalue estimates for* (4.5)—(4.6)

| $k$ | $\lambda_k$ | $\lambda_k - \tilde{\lambda}_k^{(n)}$ | | |
|---|---|---|---|---|
| | | $n=19$ | $n=39$ | $n=79$ |
| 1 | 1.5199 | .0015 | .0004 | .0000 |
| 2 | 4.9433 | .0080 | .0016 | .0004 |
| 3 | 10.2847 | .0208 | .0042 | .0009 |
| 4 | 17.5600 | .0398 | .0077 | .0017 |
| 5 | 26.7829 | .0646 | .0120 | .0025 |
| 6 | 37.9644 | .0954 | .0169 | .0034 |
| 7 | 51.1134 | .1324 | .0223 | .0042 |
| 8 | 66.2364 | .1762 | .0282 | .0050 |
| 9 | 83.3390 | .2278 | .0346 | .0059 |
| 10 | 102.4250 | .2886 | .0415 | .0066 |
| 11 | 123.4977 | .3601 | .0492 | .0075 |
| 12 | 146.5596 | .4446 | .0575 | .0086 |
| 13 | 171.6126 | .5452 | .0665 | .0092 |
| 14 | 198.6584 | .6658 | .0766 | .0100 |
| 15 | 227.6980 | .8121 | .0876 | .0109 |
| 16 | 258.7326 | .9925 | .0998 | .0118 |
| 17 | 291.7629 | 1.2204 | .1131 | .0130 |
| 18 | 326.7896 | 1.5196 | .1280 | .0138 |
| 19 | 363.8133 | 1.9145 | .1445 | .0151 |
| 20 | 402.8343 | — | .1628 | .0161 |

*The choice of* $\alpha$: As indicated in Theorem 3.1, $\alpha < 1$ and independent of $n$. On the basis of numerical experimentation, it appears that $\alpha = 1/2$ is satisfactory. This clearly illustrates the utility of the correction procedure for generating uniformly valid approximations to long sequences of eigenvalues.

## 5. Possible Generalizations

Although we will not extend the convergence bound given in Theorem 3.1, it is worthwhile noting that the above technique for correcting eigenvalue estimates can be applied to more general eigenvalue problems such as

$$-y''+q\,y=\lambda\,y,\quad y=y(x), \tag{5.1}$$

$$\sigma_1\,y(0)+\sigma_2\,y'(0)=0, \tag{5.2}$$

$$\theta_1\,y(\pi)-\theta_2\,y'(\pi)=0. \tag{5.3}$$

After using central differences to approximate $-y''$ on the grid $\boldsymbol{G}$ of (1.3), and to approximate $y'$ at the boundary, the differential eigenvalue problem (5.2)—(5.3) is replaced by the algebraic problem

$$-A\,\underline{u}+D\,\underline{u}=\lambda^{(n)}\underline{u} \tag{5.4}$$

where $D=\operatorname{diag}(q(x_1),\ldots,q(x_n))$ and

$$A=\frac{1}{h^2}\begin{Bmatrix} -2+\dfrac{2h\sigma_1}{\sigma_2} & 2 & & 0 \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \\ 0 & & -2 & 1 \\ & 1 & 2 & -2+\dfrac{2h\theta_1}{\theta_2} \end{Bmatrix}$$

With the ordered eigenvalues of (5.4) denoted by $\lambda_k^{(n)}$, $k=1,2,\ldots,n$, the corrected eigenvalue estimates are given by

$$\tilde{\lambda}_k^{(n)}=\lambda_k^{(n)}+\mu_k-\bar{\mu}_k^{(n)},\quad k=1,2,\ldots,n-1$$

where $\mu_k$, $k=1,2,\ldots$, are the eigenvalues of (5.1)—(5.3) with $q\equiv0$, and $\mu_k^{(n)}$, $k=1,2,\ldots,n$, are the eigenvalues of (5.4) with $D\equiv0$.

If we apply this technique with $n=39$ to the eigenvalue problem

$$-y''+\exp(x)\,y=\lambda\,y,\quad y=y(x), \tag{5.5}$$

$$y(0)=y'(\pi)=0, \tag{5.6}$$

then the results given in Table 5 show that the errors in the corrected estimates are superior to the original estimates. In fact, the error in the corrected estimates is uniformly bounded for the values of $k$ given.

Clearly, the above technique for correcting algebraic eigenvalues extends naturally to general differential eigenvalue problems. The actual implementation will of course depend on whether there is a simpler but related differential problem for which the eigenvalues can be determined with sufficient accuracy.

Finally, we note that the eigenvalue estimates generated by a finite element method could be improved if they were corrected using an appropriate form of the above technique. All that is required are accurate estimates of $\mu_k$, $k=1,\ldots,$ and $\mu_k^{(n)}$, $k=1,2,\ldots,n$, for a simple but related differential eigenvalue problem.

Table 5. *Error in standard and corrected eigenvalue estimates for* (5.5)—(5.6)

| $k$ | $\lambda_k$ | $\lambda_k - \lambda_k^{(n)}$ | $\lambda_k - \tilde{\lambda}_k^{(n)}$ |
|---|---|---|---|
| 1 | 4.8957 | .0029 | .0028 |
| 2 | 9.9995 | .0168 | .0142 |
| 3 | 15.4684 | .0405 | .0204 |
| 4 | 21.0369 | .0770 | .0000 |
| 5 | 28.1890 | .2031 | −.0068 |
| 6 | 37.7905 | .4641 | −.0034 |
| 7 | 49.6135 | .9086 | −.0010 |
| 8 | 63.5203 | 1.6081 | .0003 |
| 9 | 79.4643 | 2.6448 | .0010 |
| 10 | 97.4277 | 4.1118 | .0018 |
| 11 | 117.4022 | 6.1107 | .0024 |
| 12 | 139.3837 | 8.7528 | .0031 |
| 13 | 163.3697 | 12.1573 | .0038 |
| 14 | 189.3590 | 16.4515 | .0047 |
| 15 | 217.3505 | 21.6887 | .0053 |
| 16 | 247.3436 | 28.2493 | .0063 |
| 17 | 279.3380 | 36.0381 | .0073 |
| 18 | 313.3334 | 45.2844 | .0084 |
| 19 | 349.3296 | 56.1408 | .0097 |
| 20 | 387.3263 | 68.7626 | .0112 |

For example, if we use the standard linear elements on the grid $\boldsymbol{G}$ of (1.3) to approximate the eigenvalues of (1.1)—(1.2), then it follows that $\mu_k = k^2$ and

$$\mu_k^{(n)} = \frac{6(1-\cos k h)}{h^2 (2+\cos k h)}, \quad k=1, 2, \ldots, n.$$

The finite element eigenvalue estimates $\lambda_k^{(n)}$, $k=1, 2, \ldots, n$, can then be corrected as previously.

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