

Correction of Sturm-Liouville Eigenvalue Estimates

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Abstract. The error in the Sturm-Liouville eigenvalue estimates obtained by replacing the coefficient function with a piecewise constant interpolate is not uniform. In this paper we present a method for correcting these estimates to obtain a uniform approximation of all eigenvalues.

1. Introduction. The choice of numerical method for efficiently approximating a sequence of eigenvalues $\{\lambda_k\}_{k=1}^m$ of the regular Sturm-Liouville problem,

$$(1.1) \quad -\ddot{u} + qu = \lambda u, \quad u = u(x), \quad \dot{} \equiv \frac{d}{dx}, \quad x \in [0, \pi],$$

$$(1.2) \quad \alpha u(0) + \beta \dot{u}(0) = 0,$$

$$(1.3) \quad \gamma u(\pi) + \delta \dot{u}(\pi) = 0,$$

depends on the desired accuracy of the estimates and also upon the number of eigenvalues needed. When a large number of uniformly accurate eigenvalue estimates are required, it is known [7] that standard methods such as [1], [4] or [6] encounter difficulties in efficiently estimating the higher eigenvalues because the corresponding eigenfunctions are highly oscillatory.

One method which has proved useful in approximating a sequence of eigenvalues (see, e.g., [2], [5], [8]) consists of choosing a partition $\Delta_N = \{0 = x_0 < x_1 < \cdots < x_N = \pi\}$ of $[0, \pi]$ (usually uniform) and then finding the eigenvalues $\{\hat{\lambda}_k\}_{k=1}^m$ of the Sturm-Liouville problem

$$(1.4) \quad -\ddot{u} + \hat{q}u = \lambda u, \quad x \in [0, \pi],$$

$$(1.5) \quad \alpha u(0) + \beta \dot{u}(0) = 0,$$

$$(1.6) \quad \gamma u(\pi) + \delta \dot{u}(\pi) = 0,$$

obtained from (1.1)–(1.3) by replacing q by a piecewise polynomial interpolate \hat{q} on Δ_N .

The order of convergence of this method has been analyzed in [5] for piecewise constant interpolation and in [8] for general polynomial interpolation. The behavior of the error as a function of k has been analyzed in [7], where it was shown that, when Δ_N is uniform and \hat{q} is obtained using midpoint interpolation, the eigenvalue estimates satisfy

$$(1.7) \quad |\lambda_k - \hat{\lambda}_k| \leq Ch^2, \quad k = 1, 2, \dots, [N/2],$$

where $h = \pi/N$ and C is a constant bounded independently of k and h . For values

of k greater than $[N/2]$ there is a component of the error which grows rapidly as k approaches multiples of N and

$$|\lambda_k - \hat{\lambda}_k| \leq Ch, \quad k = 1, 2, 3, \dots,$$

is the best bound that is valid for all values of k .

In this paper we present a simple modification of the above method which evaluates and removes the nonuniform component of the error in $\hat{\lambda}_k$ and hence yields uniform estimates of all eigenvalues.

2. Derivation of the Correction. We restrict attention to approximating problems of the form (1.4)–(1.6), where \hat{q} is defined by

$$\hat{q}(x) = q(x_{i+1/2}), \quad x \in [x_i, x_{i+1}], \quad i = 0, 1, \dots, N - 1,$$

on the uniform partition Δ_N of $[0, \pi]$ and $x_{i+1/2} = \frac{1}{2}(x_i + x_{i+1})$. We further assume that the eigenfunction \hat{u}_k of (1.4)–(1.6), corresponding to the eigenvalue $\hat{\lambda}_k$, is normalized so that

$$\|\hat{u}_k\|_2 = \|u_k\|_2 = 1 \quad \text{and} \quad \int_0^\pi u_k \hat{u}_k \, dx > 0.$$

In order to derive the required correction factor and to establish the uniformity of the error in the corrected eigenvalue estimates, we firstly state some results derived in [7].

LEMMA 2.1. *Let $q \in C^2[0, \pi]$, $f \in C^1[0, \pi]$ and \hat{q} be the midpoint interpolate of q on the uniform partition Δ_N of $[0, \pi]$. Then*

$$\left| \int_0^\pi (q - \hat{q})f \, dx \right| \leq \pi \left\{ \frac{1}{4} \|q'\|_\infty \|f'\|_\infty + \frac{1}{8} \|q''\|_\infty \|f\|_\infty \right\} h^2.$$

LEMMA 2.2. *Let the conditions of Lemma 2.1 be satisfied and define*

$$\rho = \frac{1}{2} \min_k |\lambda_{k+1} - \lambda_k|.$$

Then

$$(2.1) \quad \begin{aligned} \left| \lambda_k - \hat{\lambda}_k - \int_0^\pi (q - \hat{q})u_k^2 \, dx \right| &\leq 4\rho^{-1} \|q - \hat{q}\|_\infty^2, & k = 1, 2, 3, \dots, \\ &\leq \rho^{-1} \|q'\|_\infty^2, \end{aligned}$$

if $\|q - \hat{q}\|_\infty < \frac{1}{2}\rho$.

Lemma 2.2 indicates that there are two (not independent) principal components which comprise the error $|\lambda_k - \hat{\lambda}_k|$. The first, $4\rho^{-1} \|q - \hat{q}\|_\infty^2$, is due to approximating q with a piecewise constant interpolate and is independent of k . The second, $|\int_0^\pi (q - \hat{q})u_k^2 \, dx|$, is the error in evaluating $\int_0^\pi qu_k^2 \, dx$ using product midpoint quadrature, and obviously depends on k . To examine this dependence we note [3, p. 336] that $u_k = v_k + O(k^{-1})$, where $v_k = A_k \sin(\mu_k x + \phi_k)$ is the eigenfunction of (1.1)–(1.3) with $q \equiv 0$, corresponding to the eigenvalue μ_k and normalized in the same manner as \hat{u}_k . This asymptotic result used in conjunction with Lemma 2.1 gives

$$(2.2) \quad \left| \int_0^\pi (q - \hat{q})u_k^2 \, dx \right| \leq \left| \int_0^\pi (q - \hat{q})v_k^2 \, dx \right| + Ch^2.$$

On noting that $\mu_k = k + O(1)$, a further application of Lemma 2.2 with $f = v_k^2$ yields

$$\left| \int_0^\pi (q - \hat{q}) v_k^2 dx \right| \leq C_2 k h^2$$

and hence, from (2.1) and (2.2),

$$(2.3) \quad |\lambda_k - \hat{\lambda}_k| \leq C_1 h^2 + C_2 k h^2,$$

where C_1 and C_2 depend only on q .

Examining this dependence on q further, we see that if q is a rapidly varying function, then the smallest value of N which will make the component $4\rho^{-1} \|q - \hat{q}\|_\infty^2$ sufficiently small to give the desired accuracy in the eigenvalue estimates will probably be large enough so that (1.7) will guarantee uniformity of the error for the eigenvalues required. However, if q is only slowly varying or if a particularly long sequence of eigenvalues are required, then this value of N may not be large enough in order to apply (1.7), and the growth exhibited in (2.3) may become apparent in the estimates.

In the latter case one could simply take N to be at least twice the number of eigenvalues required, however, if we can (uniformly) estimate the component of the error which grows with k , then a potentially more efficient approach would be to correct the eigenvalues using this information and hence obtain uniform estimates.

Returning to (2.1), we see that the component of the error that grows with k depends on u_k (the exact eigenfunction) and so cannot be estimated directly. But if we use (2.2), (2.1) can be replaced by

$$(2.4) \quad \left| \lambda_k - \hat{\lambda}_k - \int_0^\pi (q - \hat{q}) v_k^2 dx \right| \leq C h^2, \quad k = 1, 2, 3, \dots$$

Since q , \hat{q} and v_k are known functions, we could now apply a standard quadrature rule to evaluate $\int_0^\pi (q - \hat{q}) v_k^2 dx$, except that we would still face the problem of uniformly estimating the integral because of its dependence on v_k . However, if we note that

$$|q(x) - q(x_{i+1/2}) - q_h(x)| \leq C h^2, \quad x \in [x_i, x_{i+1}],$$

where $q_h(x) = h^{-1}(x - x_{i+1/2})(q_{i+1} - q_i)$ and $q_i = q(x_i)$, then obviously $\|q - \hat{q} - q_h\|_\infty \leq C h^2$ and hence

$$(2.5) \quad \begin{aligned} \left| \int_0^\pi (q - \hat{q}) v_k^2 dx \right| &\leq \left| \int_0^\pi q_h v_k^2 dx \right| + \left| \int_0^\pi (q - \hat{q} - q_h) v_k^2 dx \right| \\ &\leq \left| \int_0^\pi q_h v_k^2 dx \right| + \|q - \hat{q} - q_h\|_\infty \|v_k\|_2^2 \leq \left| \int_0^\pi q_h v_k^2 dx \right| + C h^2. \end{aligned}$$

Since q_h is a piecewise linear polynomial and v_k is a trigonometric function, the integral $\int_0^\pi q_h v_k^2 dx$ can now be evaluated exactly, and we have

$$\begin{aligned} \int_0^\pi q_h v_k^2 dx &= \frac{1}{2} A_k^2 \left\{ \int_0^\pi q_h dx - \int_0^\pi q_h \cos 2(\mu_k x + \phi_k) dx \right\} \\ &= \frac{1}{2} h A_k^2 \left\{ \frac{\sin \mu_k h}{\mu_k h^2} - \frac{\cos \mu_k h}{\mu_k h} \right\} \sum_{i=0}^{N-1} (q_{i+1} - q_i) \sin 2(\mu_k x_{i+1/2} + \phi_k) \end{aligned}$$

since $\int_0^\pi q_h dx = 0$.

In summary then we have

THEOREM 2.1. *Let the conditions of Lemmas 2.1 and 2.2 be satisfied. Then,*

$$|\lambda_k - \bar{\lambda}_k| \leq Ch^2, \quad k = 1, 2, 3, \dots,$$

where

$$(2.6) \quad \bar{\lambda}_k = \hat{\lambda}_k + \int_0^\pi q_h v_k^2 dx$$

and C is bounded independently of k and h .

Proof. This result follows directly from (2.4) and (2.5).

3. A Numerical Example. To illustrate the improvement of the eigenvalue estimates which can be obtained by using the corrected estimates (2.6), we calculated $\{\hat{\lambda}_k\}_{k=1}^{40}$ for the eigenvalue problem

$$(3.1) \quad -\ddot{u} + e^x u = \lambda u, \quad x \in [0, 1], u(0) = 0 = u(1),$$

with $N = 16$. The error in these estimates is plotted against k in Figure 3.1 and clearly shows both the uniformity of the error for $k < N/2$ and also the growth as k approaches multiples of N . If we now use (2.6) to generate the corrected estimates, then the error, shown in Figure 3.2, is obviously superior to the error in the uncorrected estimates and can be seen to achieve the desired uniformity.

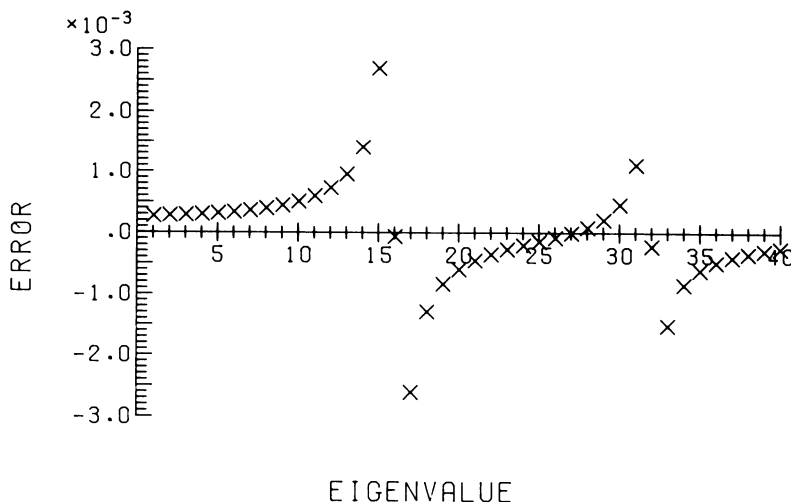


FIGURE 3.1

Eigenvalue error for (3.1) obtained by approximating the differential equation

The reason for the anomalous behavior of the error for $k = 16$ and 32 (i.e. multiples of N) is not clear, though it should be noted that this behavior is not in conflict with the bound given in Theorem 2.1.

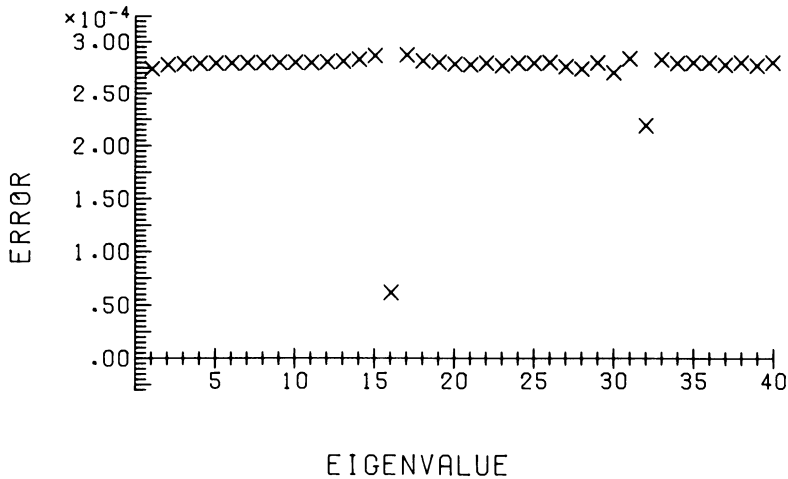


FIGURE 3.2

Eigenvalue error in using (2.6) to correct the eigenvalue estimates

4. Conclusion. In approximating Sturm-Liouville eigenvalues, the growth of the error with k often reflects the increasingly oscillatory behavior of the eigenfunctions rather than any difficulty caused by the particular coefficient function. In this paper we have identified, and shown how to remove, this nonuniform component of the error for one particular method for approximating eigenvalues. Thus, for any given Sturm-Liouville eigenvalue problem, the difficulty in obtaining acceptable estimates of a sequence of eigenvalues using this corrected method will be solely due to the characteristics of the coefficient function rather than the number of eigenvalues required.

This method of correcting the eigenvalue estimates by evaluating and removing the dominant k -dependent component of the error should also be applicable to the more general methods given in [8], where q is approximated by a piecewise polynomial of degree $n \geq 1$. Though in this case the remaining error terms will still depend on k , and hence the effect of the correction will be to reduce the rate of growth of the error rather than to eliminate it altogether.

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1. G. BIRKHOFF, C. DE BOOR, B. SWARTZ & B. WENDROFF, "Rayleigh-Ritz approximation by piecewise polynomials," *SIAM J. Numer. Anal.*, v. 3, 1966, pp. 188-203.
2. J. CANOSA & R. GOMES DE OLIVEIRA, "A new method for the solution of the Schrödinger equation," *J. Comput. Phys.*, v. 5, 1970, pp. 188-207.
3. R. COURANT & D. HILBERT, *Methods of Mathematical Physics*, Vol. I, Interscience, New York, 1953.

4. B. HUBBARD, "Bounds for eigenvalues of the Sturm-Liouville problem by finite difference methods," *Arch. Rational Mech. Anal.*, v. 10, 1962, pp. 171–179.
5. L. GR. IXARU, "The error analysis of the algebraic method for solving the Schrödinger equation," *J. Comput. Phys.*, v. 9, 1972, pp. 159–163.
6. H. B. KELLER, *Numerical Methods for Two-point Boundary Value Problems*, Blaisdell, Waltham, Mass., 1968.
7. J. W. PAINE & F. R. DE HOOG, "Uniform estimation of the eigenvalues of Sturm-Liouville problems," *J. Austral. Math. Soc. Ser. B*, v. 21, 1980, pp. 356–383.
8. S. PRUESS, "Estimating the eigenvalues of Sturm-Liouville problems by approximating the differential equation," *SIAM J. Numer. Anal.*, v. 10, 1973, pp. 55–68.