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Leighton's Bounds for Sturm–Liouville Eigenvalues

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An error is pointed out in a method of W. Leighton for computing two-sided bounds for the eigenvalues of the Sturm–Liouville problem $(ry')' + \lambda py = 0$, $y(a) = y(b) = 0$. The error is corrected, the underlying theory is examined and the method is generalized.

1. INTRODUCTION

Leighton [3] has suggested a simple numerical method for computing two-sided bounds for the eigenvalues of the Sturm–Liouville problem

$$(ry')' + \lambda py = 0, \tag{1.1a}$$

$$y(a) = y(b) = 0, \tag{1.1b}$$

where r and p are continuous and positive on $[a, b]$. Leighton's idea was to divide $[a, b]$ into n subintervals and on each subinterval solve the equation with p and r replaced by constants. In addition to (1.1b), boundary conditions are imposed at the ends of the subintervals by imposing certain continuity conditions on y. Similar ideas have been used by others ([4] and the references given there) to obtain estimates, but, except in [1], not bounds, for eigenvalues. Leighton illustrated his ideas by a numerical example with the interval divided into four subintervals.

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In this paper, an important error in [3] is pointed out. It is shown that when, in Leighton's numerical example, the number of subintervals is increased, the upper bounds given by his Eq. (2.9) (subsequently referred to as (L2.9)) become lower than the true eigenvalues. This error is corrected, the underlying theory is examined and the method is generalized.

The error arises from Leighton's choice of continuity conditions for y. He imposes the condition

$$y \in C^1[a, b]. \tag{1.2}$$

It is shown in Section 2 that the appropriate condition to impose on the solution of (1.1) when r has jump discontinuities is

$$y \in C[a, b], \qquad ry' \in C[r; a, b], \tag{1.3}$$

where the notation $u \in C[r; a, b]$ means that there exists a function $u_1 \in C[a, b]$ such that $u(x) = u_1(x)$ for all $x \in [a, b]$ except perhaps the points of discontinuity of r. In general, y' will not exist at jump discontinuities of r. The error in [3] may have arisen because (L2.9) is derived for the special case when $r \equiv 1$ and then used (p. 386), without the appropriate modifications (see Section 3 below), for problems with a non-constant r. This difficulty does not affect the work of Day [1], who, like many others, considered only the Liouville normal form (in which $r \equiv 1$).

2. Theory

Leighton stated that his Theorem 3.1 was an immediate consequence of the Sturm–Picone theorem and that this theorem remained valid when r and p have a finite number of finite discontinuities. Since most references consider only the case $r \in C[a, b]$ (when (1.2) and (1.3) are identical), the relevant theory is developed here for completeness.

We first introduce some notation. Let $x_0 < x_1 < \cdots < x_m$ and let $PC[x_0, x_m]$ denote the class of functions in

$$C[x_0, x_1) \cap C(x_1, x_2) \cap \cdots \cap C(x_{m-1}, x_m]$$

for which left and right hand limits exist at $x_1, \ldots, x_{m-1}$.

Theorem 2.1. *For $j = 1, 2$ let*

(i) $r_j, r_j', q_j \in PC[x_0, x_m]$;

(ii) $y_j \in C[x_0, x_m]$, $r_j y_j' \in C[r_j; x_0, x_m]$;

(iii) $(r_j y_j')' + q_j y_j = 0$ *on* (x_{i-1}, x_i), $i = 1, \ldots, m$;

(iv) $y_j(x_0) = \alpha_j$, $(r_j y_j')(x_0) = \beta_j$, $|\alpha_j| + |\beta_j| > 0$;

(v) $r_1 \geqslant r_2 \geqslant r_0$ *(const.)* > 0, $q_2 > q_1$ *on* (x_{i-1}, x_i), $i = 1,\ldots, m$; *and*

(vi) *if* $\alpha_1 \neq 0$, *then* $\alpha_2 \neq 0$ *and* $\beta_1/\alpha_1 \geqslant \beta_2/\alpha_2$.

Let y_1 *have* k $(\geqslant 0)$ *zeros in* $(x_0, x_m]$. *Then* y_2 *has at least* k *zeros in* $(x_0, x_m]$ *and the sth* $(s \leqslant k)$ *zero of* y_2 *is less than the sth zero of* y_1. *Furthermore, if* y_1 *and* y_2 *have the same number of zeros in* (x_0, x_m) *then* $y_1(x_m) \neq 0$ *and if in addition* $y_2(x_m) \neq 0$, *then* $(r_1 y_1'/y_1)(x_m) > (r_2 y_2'/y_2)(x_m)$.

Proof. Induction on m shows that this follows from the first and second comparison theorems for the continuous case as given in Ince [2, pp. 228, 229]. ∎

THEOREM 2.2. *For* $j = 1, 2$, *let*

(i) $r_j, r_j', p_j, q_j \in PC[x_0, x_m]$;

(ii) $y_j \in C[x_0, x_m]$, $r_j y_j' \in C[r_j; x_0, x_m]$;

(iii) $(r_j y_j')' + (\lambda^{(j)} p_j - q_j) y_j = 0$ *on* (x_{i-1}, x_i), $i = 1,\ldots, m$;

(iv) $\alpha_j(r_j y_j')(x_0) = \beta_j y_j(x_0)$, $|\alpha_j| + |\beta_j| > 0$, $\gamma_j(r_j y_j')(x_m) = \delta_j y_j(x_m)$, $|\gamma_j| + |\delta_j| > 0$;

(v) $p_2 \geqslant p_1 \geqslant p_0$ *(const.)* > 0, $r_1 \geqslant r_2 \geqslant r_0$ *(const.)* > 0 *and* $q_1 \geqslant q_2$ *on* (x_{i-1}, x_i), $i = 1,\ldots, m$;

(vi) *if* $\alpha_1 \neq 0$, *then* $\alpha_2 \neq 0$ *and* $\beta_1/\alpha_1 \geqslant \beta_2/\alpha_2$; *and*

(vii) *if* $\gamma_1 \neq 0$, *then* $\gamma_2 \neq 0$ *and* $\delta_1/\gamma_1 \leqslant \delta_2/\gamma_2$.

Then,

(a) *the above eigenvalue problems each have a countable infinity of eigenvalues* $\lambda_1^{(j)} \leqslant \lambda_2^{(j)} \leqslant \cdots$ *and the eigenfunction corresponding to* $\lambda_k^{(j)}$ *has exactly* $(k-1)$ *zeros in* (x_0, x_m), *and*

(b) $\lambda_k^{(1)} \geqslant \lambda_k^{(2)}$ *for all* $k \in \mathbf{N}$ *for which* $\lambda_k^{(1)}(p_1 - p_2) \leqslant 0$.

Proof. (a) The proof is the same as that of Theorem II in Ince [2, p. 233] except that it uses Theorem 2.1 above instead of Sturm's original comparison theorems.

(b) Suppose $\lambda_k^{(1)} < \lambda_k^{(2)}$ although $\lambda_k^{(1)}(p_1 - p_2) \leqslant 0$. Then $(\lambda_k^{(1)} p_1 - q_1) - (\lambda_k^{(2)} p_2 - q_2) = (\lambda_k^{(1)} - \lambda_k^{(2)}) p_2 + \lambda_k^{(1)}(p_1 - p_2) + q_2 - q_1 < 0$. Hence, it follows from (a) and Theorem 2.1 that $y_k^{(1)}$ and $y_k^{(2)}$ cannot both satisfy the boundary conditions. ∎

The condition $\lambda_k^{(1)}(p_1 - p_2) \leqslant 0$, required in Theorem 2.2b, is satisfied if at least one of the following is true:

(i) $p_1 = p_2$ (as in all problems in Liouville normal form) or

(ii) $\lambda_k^{(1)} \geqslant 0$.

The latter condition is satisfied for all k if, for example, $q_1 \geqslant 0$ and $\alpha_1 \beta_1 \geqslant 0 \geqslant \gamma_1 \delta_1$, as is the case in (1.1). A similar proof shows $\lambda_k^{(2)} \geqslant 0$ to be a sufficient condition.

Discussion of the algorithm is facilitated by yet more notation. Let

$$R_i^+ = \sup_{(x_{i-1}, x_i)} r, \qquad R_i^- = \inf_{(x_{i-1}, x_i)} r,$$

and

$$r^+(x) = R_i^+ \qquad \text{when } x_{i-1} < x \leqslant x_i,\ i = 1,\dots, n \text{ with } r^+(x_0) = R_1^+,$$

and define numbers P_i^+, P_i^-, Q_i^+ and Q_i^- and functions r^-, p^+ and p^- similarly. In Leighton's method, (1.1a) is replaced by

$$(R_i y')' + \lambda P_i y = 0 \qquad \text{on } (x_{i-1}, x_i),\ i = 1,\dots, n, \tag{2.1}$$

where $a = x_0 < x_1 < \cdots < x_n = b$. Theorem 2.2 shows that (2.1), with boundary conditions given by (1.1b) and (1.3), will give lower bounds, λ_k^-, for the eigenvalues, λ_k, of (1.1) if

$$R_i = R_i^-, \qquad P_i = P_i^+, \qquad i = 1,\dots, n, \tag{2.2a}$$

and upper bounds, λ_k^+, if instead

$$R_i = R_i^+, \qquad P_i = P_i^-, \qquad i = 1,\dots, n. \tag{2.2b}$$

Indeed since

$$0 < \rho_3 r \leqslant r^- \leqslant r \leqslant r^+ \leqslant \rho_1 r \qquad \text{and} \qquad 0 < \rho_4 p \leqslant p^- \leqslant p \leqslant p^+ \leqslant \rho_2 p,$$

where

$$\rho_1 = \sup_{[a,b]} r^+/r, \qquad \rho_2 = \sup_{[a,b]} p^+/p,$$

$$\rho_3 = \inf_{[a,b]} r^-/r, \qquad \rho_4 = \inf_{[a,b]} p^-/p,$$

Theorem 2.2 shows that, for all $k \in \mathbf{N}$,

$$\rho_1 \lambda_k/\rho_4 \geqslant \lambda_k^+ \geqslant \lambda_k \geqslant \lambda_k^- \geqslant \rho_3 \lambda_k/\rho_2. \tag{2.3}$$

If p and r are continuous (or even in $PC[x_0, x_m]$ for some fixed partition, $a = x_0 < x_1 < \cdots < x_m = b$) and bounded away from zero then $\rho_j \to 1$, $j = 1,\dots, 4$, as the partition is refined with $\max |x_i - x_{i-1}| \to 0$. Convergence of the bounds follows from (2.3). Indeed Taylor's theorem shows that if n equal subintervals are used and p and r are in $C^1[a, b]$, then $\rho_j = 1 + O(n^{-1})$,

$j = 1,..., 4$ so that in this case convergence of λ_k^+ and λ_k^- to λ_k is of order n^{-1}. Theorem 2.2 also shows that for successive refinements of the partition of $[a, b]$ the convergence is monotonic. Analogous results may be proved for the more general problem considered in Section 3.

Similar arguments show that if (as recommended in [3]) the boundary conditions (1.1b) and (1.2) are used, then the eigenvalues of (2.1) will converge, as $\max_i |x_i - x_{i-1}| \to 0$, to the eigenvalues of

$$ry'' + \lambda py = 0, \qquad y(a) = y(b) = 0. \tag{2.4}$$

Applying the transformation $y = r^{-1/2}u$ to (1.1) then shows that whenever $(r^{-1/2}r')' > 0$, a condition satisfied by Leighton's numerical example, the "upper" bounds given by his algorithm will be lower than the true eigenvalue whenever $\max_i |x_i - x_{i-1}|$ is sufficiently small.

In [3] Leighton used similar ideas to obtain bounds for conjugate points. When the method is used for this purpose, Theorem 2.1 shows that the continuity requirement is again (1.3) and not (1.2). This does not affect the single numerical example given in [3, Sect. 4] as this has $r \equiv 1$.

3. The Modified Algorithm

Consider the eigenvalue problem

$$(ry')' + (\lambda p - q)y = 0 \qquad \text{on } (x_{i-1}, x_i),\ i = 1,..., n, \tag{3.1a}$$

$$\begin{gathered} \alpha(ry')(x_0) + \beta y(x_0) = \gamma(ry')(x_n) + \delta y(x_n) = 0, \\ |\alpha| + |\beta| > 0, \qquad |\gamma| + |\delta| > 0, \end{gathered} \tag{3.1b}$$

$$r, r', p, q \in PC[x_0, x_n], \quad y \in C[x_0, x_n], \quad ry' \in C[r; x_0, x_n], \tag{3.1c}$$

where $r \geqslant r_0$ (const.) > 0, $p \geqslant p_0$ (const.) > 0 on $[x_0, x_n]$. Theorem 2.2(b) may be used to give bounds for the kth eigenvalue, λ_k, of (3.1) whenever at least one of the following conditions is satisfied:

(i) $p \equiv 1$ (as in all problems in Liouville normal form) or

(ii) $\lambda_k \geqslant 0$ or

(iii) the kth zero of (3.2) below is nonnegative.

This requirement, which is satisfied for all k in the special cases studied in [1, 3], is assumed henceforth.

Using calculations analogous to those in [1, 3] it can be deduced from Theorem 2.2 that a lower bound for λ_k will be given by the kth zero of

$$f(\lambda) = 0, \tag{3.2a}$$

where

$$\begin{aligned} f(\lambda) &= \gamma c_n[1 - z_n \tan w_n] + \delta[z_n + \tan w_n], && \text{if} \quad \lambda P_n > Q_n, \\ &= \gamma c_n[1 + z_n \tanh w_n] + \delta[z_n + \tanh w_n], && \text{if} \quad \lambda P_n < Q_n, \end{aligned} \tag{3.2b}$$

and, for $i = 2,..., n-1$,

$$\begin{aligned} z_{i+1} &= \frac{c_{i+1}(z_i + \tan w_i)}{c_i(1 - z_i \tan w_i)}, && \text{if} \quad \lambda P_i > Q_i, \\ &= \frac{c_{i+1}(z_i + \tanh w_i)}{c_i(1 + z_i \tanh w_i)}, && \text{if} \quad \lambda P_i < Q_i, \end{aligned} \tag{3.2c}$$

and

$$\begin{aligned} z_2 &= \frac{c_2(\beta \tan w_1 - \alpha c_1)}{c_1(\beta + \alpha c_1 \tan w_1)}, && \text{if} \quad \lambda P_1 > Q_1, \\ &= \frac{c_2(\beta \tanh w_1 - \alpha c_1)}{c_1(\beta - \alpha c_1 \tanh w_1)}, && \text{if} \quad \lambda P_1 < Q_1, \end{aligned} \tag{3.2d}$$

where, for $i = 1,..., n$,

$$c_i = |R_i(\lambda P_i - Q_i)|^{1/2} \quad \text{and} \quad w_i = c_i(x_i - x_{i-1})/R_i, \tag{3.2e}$$

when, in the notation of Section 2,

$$R_i = R_i^-, \qquad Q_i = Q_i^-, \qquad P_i = P_i^+, \qquad i = 1,..., n. \tag{3.3}$$

Similarly it can be deduced from Theorem 2.2 that if (3.3) is replaced by

$$R_i = R_i^+, \qquad Q_i = Q_i^+, \qquad P_i = P_i^-, \qquad i = 1,..., n, \tag{3.4}$$

then the kth zero of (3.2) will give an upper bound for λ_k. The (very rare) circumstance $\lambda P_i = Q_i$ can be handled by making a small perturbation of the trial value of λ in the iterative solution of (3.2), as recommended in [5] for the special case given in [1].

Clearly (1.1) is the special case of (3.1), with $r, p \in C[x_0, x_n]$, obtained by putting $q \equiv 0$ and $\alpha = \gamma = 0$. Leighton also made the restriction $x_i - x_{i-1} = (x_n - x_0)/n$, $i = 1,..., n$. Equation (3.2) simplifies in this case, but not to (L2.9), which lacks a factor R_i/R_{i-1} in the equation for z_i, $i = 2,..., n$. (Note that only the first alternative in (3.2b)–(3.2d) is needed in this case since $q \equiv 0 < \lambda p$.)

The use of an arbitrary partition here adds some flexibility to the scheme. It is immediately applicable to the case in which p, q and r have a finite number of jump discontinuities as these discontinuities may be chosen as grid points, x_i. Moreover if (as is the case in most applications) p, q and r are piecewise monotonic, the x_i may be chosen so that p, q and r are all monotonic on each subinterval (x_{i-1}, x_i), thereby greatly simplifying the calculation of P_i, Q_i and R_i.

4. Numerical Results

Leighton's numerical results concerned the eigenvalue problem

$$\begin{gathered} ((2x+1)^{-1}y')' + \lambda(2x+1)y = 0, \\ y(0) = y(1) = 0. \end{gathered} \tag{4.1}$$

In Table I, bounds for the first and fourth eigenvalues of (4.1) given by (L2.9) and by (3.2) with $n = 4$, 16, 64, 256 and 1024 equal subintervals are compared. Note that results given by (L2.9) with $n = 4$ agree with those given in [3]. Spurious bounds are marked *.

The two-sided bounds obtained by (3.2) have two important advantages over those obtained by many other methods. As predicted by (2.3), their relative accuracy (though not their absolute accuracy) is approximately the same for all eigenvalues (whereas many methods give much less accuracy for higher eigenvalues) and the true eigenvalue is close to the average of the upper and lower bounds, especially when the grid spacing is small. Although

TABLE I

Bounds for Eigenvalues of (4.1) from (3.2) and (L2.9)

n	4	16	64	256	1024
		$\lambda_1 = \pi^2/4 = 2.46740110027233965...$			
(3.2)	1.9496	2.3201	2.4293	2.45779	2.464993
	3.2227	2.6292	2.5064	2.47707	2.469812
(L2.9)	1.8330	2.1687	2.2646	2.28947	2.295737
	2.9200	2.4370*	2.3317*	2.30623*	2.299925*
		$\lambda_4 = 4\pi^2 = 39.478417604357434...$			
(3.2)	31.193	37.122	38.869	39.3247	39.43989
	51.564	42.066	40.103	39.6331	39.51700
(L2.9)	32.313	36.857	38.589	39.0377	39.15098
	52.036	41.710	39.801	39.3407*	39.22673*

the difference between the upper and lower bounds is of order n^{-1} (with n equal subintervals), the difference between the mean, $\mu_k(n)$, of the upper and lower bounds and the eigenvalue, λ_k, which they bound is of order n^{-2}. Indeed Table II indicates that the error in the estimates

$$\nu_k(n) = |16\mu_k(4n) - \mu_k(n)|/15,$$

obtained by h^2-extrapolation, is of order n^{-4}, with $\lambda_k > \nu_k(n)$ in each case computed.

Table II was compiled from bounds computed to 15 significant figures using double precision (18*D*) arithmetic on the DEC10 computer at La Trobe University, although, for ease of tabulation, only the most significant figures are shown in Table I. Since all results repeated in single precision (8*D*) showed no change in the first 7 significant figures, all 15 figures of the double precision results may be assumed correct.

Leighton also gave estimates for the first nine eigenvalues of (4.1) obtained by (L2.9) with $a_i^2 = P_i/R_i$, where

$$P_i = p\left(\frac{x_{i-1}+x_i}{2}\right), \qquad R_i = r\left(\frac{x_{i-1}+x_i}{2}\right). \tag{4.2}$$

Again the appropriate condition is not (1.2) but (1.3), which again leads to (3.2) with P_i and R_i given by (4.2) (and of course $Q_i = \alpha = \gamma = 0$). Using this formula, we obtained an astonishing 13 correct significant figures in the estimates of the first five eigenvalues using only four equal subintervals. The accuracy obtained with (4.2) in this case is not likely to be typical since it exceeds accuracy reported by others using similar methods. Nevertheless the contrast with Table II of [3] is remarkable.

Bounds given by (3.2) and by (L2.9) for the first five eigenvalues of (4.1) and of some other cases of (1.1) are given (to five significant figures) in [5], where they are compared with bounds obtained by some other methods. See also [6].

TABLE II

Errors, $\lambda_k - \nu_k(n)$, in Extrapolated Estimates

	n			
k	4	16	64	256
1	$1.927E-4$	$7.364E-7$	$2.873E-9$	$1.122E-11$
4	$3.083E-3$	$1.178E-5$	$4.596E-8$	$1.795E-10$

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