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Computational Procedure for Sturm–Liouville Problems

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The approaches of Datzeff (*C. R. Acad. Bulg. Sci.* **12** (1959), 113, 285) and Wittrick and Williams (*Quart. J. Mech. Appl. Math.* **XXIV** (1971), 263; *Int. J. Mech. Sci.* **16** (1974), 209) have been incorporated to develop a procedure for the automatic computation of the eigenvalues and the eigenfunctions of one-dimensional linear Sturm–Liouville boundary value eigenproblems, both singular and nonsingular. The continuous coefficients of a regular Sturm–Liouville problem have been approximated by a finite number of step functions. In each step the resulting boundary value problem has been integrated exactly and the solutions have then been matched to construct the continuously differentiable solution of the original problem and the corresponding eigencondition. Step sizes have been chosen automatically so that the local error has been held in a predetermined interval. Representative test examples have been computed to illustrate the accuracy, reliability, and efficiency of the algorithm proposed.

1. INTRODUCTION

The solution of various problems in the field of mathematical physics and engineering is closely related to the solution of the corresponding one-dimensional linear Sturm–Liouville boundary value eigenproblem. As particular examples, one could imagine the one-dimensional Schrödinger equation with space-dependent potential function and numerous problems of physico-chemical kinetics [5].

A number of methods have been developed to solve one-dimensional Sturm–Liouville problems, among these finite difference methods [6, 7], imbedding techniques [8], and shooting type procedures [9, 10] based on integrators for systems of ordinary differential equations. Regardless of the particular method utilized, one always has difficulties with the computation of the higher-order eigenvalues and eigenfunctions due to their rapid oscillation character. This results in the need for finer interval of integration resolution, thus making the computer time involved unreasonable.

Recently Hargrave [11] and Bailey [12, 13] proposed to solve linear Sturm–Liouville eigenproblems utilizing a Prüffer transformation of the original problem. This turned out to be helpful because the approach allowed one to compute the eigenvalues solving only one ordinary differential equation numerically. Moreover, in the corresponding initial value problem the order of the eigenvalue was present explicitly, thus making the computational procedure safe from missing eigenvalues. One other

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feature of the method discussed is that the general purpose integrators are safer when applied to the phase function instead of being applied directly on the eigenfunction [12]. After analyzing in detail the integration methods available to solve numerically Sturm–Liouville eigenproblems, Bailey developed a general purpose solver based on the Prüffer transformation that was tested on a number of examples [12, 13].

In [1, 2] Datzeff developed a method enabling one to obtain principally an approximation of the whole infinite spectrum of the one-dimensional linear space-dependent Schrödinger equation. A stepwise approximation of the external potential function was applied, thus replacing the original problem with a sequence of finite sets of Sturm–Liouville problems with constant coefficients defined on subintervals of the initial interval of integration. He also proved that the spectra of the approximate problems tend to the spectrum of the original problem as the length of the largest subinterval tends to zero. Any such approximation of the original problem can be integrated exactly in terms of circular and hyperbolic functions. The solutions defined on consequent subintervals can then be matched at the corresponding interfaces to ensure continuous differentiability of the solution of the approximate problem and to derive the eigencondition of the problem. Such an approach guarantees roughly the same accuracy of the ground and the higher-order eigenvalues and eigenfunctions. These papers were published at the beginning of the computer era and thus no numerical examples were presented to illustrate the computational advantages of this method.

The same approach was later developed by Canosa and Oliveira [14]. They illustrated its efficiency by many numerical examples. The method was tested again by Canosa [15] to show its applicability for some practically asymptotic problems. A trial and error procedure was used to locate the eigenvalues, based on the computation of $\det[K(\lambda)]$ for randomly chosen values of λ and simply observing where the determinant changed sign. Such a procedure, however, is generally not safe from missing eigenvalues in the course of the computation.

Wittrick and Williams [3, 4] developed an extremely efficient algorithm (in terms of computer time) for the safe and automatic computation of the natural frequencies and buckling loads of linear elastic skeletal structures. It permits one to estimate exactly how many natural frequencies lie below any fixed value of the frequency parameter without calculating them explicitly, thus being able to obtain upper and lower bounds for any required eigenfrequency to any desired accuracy.

Purpose of the present paper is to combine the approaches of Datzeff and of Wittrick and Williams to develop a computational procedure for the solution of one-dimensional linear Sturm–Liouville boundary value eigenproblems. The applicability of the algorithm will be demonstrated by recalculating several problems previously published.

2. Statement and Analytical Aspects of the Problem

The present discussion concerns the one-dimensional linear Sturm–Liouville boundary value eigenproblem

$$(d/dx)(p(x)(d/dx)\,\Psi(x,\Lambda)) + (\Lambda r(x) - q(x))\,\Psi(x,\Lambda) = 0, \qquad a < x < b, \quad (1a)$$

$$\alpha_0\,\Psi(x,\Lambda) - \beta_0\,p(x)(d/dx)\,\Psi(x,\Lambda) = 0, \qquad x = a, \quad (1b)$$

$$\alpha_n\,\Psi(x,\Lambda) + \beta_n\,p(x)(d/dx)\,\Psi(x,\Lambda) = 0, \qquad x = b, \quad (1c)$$

where the constants α_0, β_0, α_n, and β_n are real and independent of the parameter Λ.

A linear boundary value problem described by equations such as (1a)–(1c) is said to be regular [11–13] when:

(a) $[a, b]$ is finite,

(b) $p(x)$, $r(x)$, and $q(x)$ are continuous in $[a, b]$,

(c) $p(x)$ is continuously differentiable in $[a, b]$, and

(d) $p(x)$ and $r(x)$ are positive in $[a, b]$.

If one or more of conditions (a)–(d) are violated, the problem is said to be singular.

Let the coefficients $p(x)$, $r(x)$, and $q(x)$ be approximated by stepwise functions as

$$p(x) = p_k, \qquad r(x) = r_k, \qquad q(x) = q_k$$

for $x_{k-1} < x < x_k$, $k = 1, 2,..., n$, $x_0 = a$, $x_n = b$. This choice of the approximation of the coefficients is convenient in utilizing the standard mathematical functions present in practically all kinds of digital computers [16]. In this way even a regular problem like Eqs. (1a)–(1c) is replaced by a singular one. The values of the constants p_k, r_k, and q_k, $k = 1, 2,..., n$, can be chosen in various manners; they can be taken as the values of the coefficients $p(x)$, $r(x)$, and $q(x)$ at the midpoints of the corresponding subintervals l_k, $l_k = x_k - x_{k-1}$, or they can be estimated as the (eventually weighted) average of the values of the coefficients at the endpoints of the subinterval as in [14, 15]. Here the division of the original interval into subintervals is taken for granted, while in a later section a procedure will be described to solve this problem.

In any of the subintervals $l_k = x_k - x_{k-1}$, $k = 1, 2,..., n$, Eq. (a) can be replaced by an equation of the kind

$$(d^2\psi_k(x,\lambda)/dx^2) + \omega_k^2\psi_k(x,\lambda) = 0, \qquad x_{k-1} < x < x_k, \quad (3a)$$

where

$$\omega_k^2 = (\lambda r_k - q_k)/p_k, \qquad k = 1, 2,..., n. \quad (3b)$$

It is seen that the coefficients in Eq. (3a) satisfy the regularity requirements in the interior of the corresponding subinterval except possibly at some endpoint, a case to be discussed in what follows.

If one imposes the restriction that $\Psi(x, \Lambda)$ has a continuous first derivative in the interior of the original interval of integration, then one has to match the eigenfunction and its first derivative at the endpoints of the corresponding subintervals, thus

$$\psi_k(x, \lambda) = \psi_{k+1}(x, \lambda), \qquad x = x_k, \quad k = 1, 2, \ldots, n-1, \tag{3c}$$

$$p_k(d\psi_k(x, \lambda)/dx) = p_{k+1}(d\psi_{k+1}(x, \lambda)/dx), \qquad x = x_k, \quad k = 1, 2, \ldots, n-1, \tag{3d}$$

while Eqs. (1b) and (1c) take the form

$$\alpha_0 \psi_1(x, \lambda) - \beta_0 p_1(d\psi_1(x, \lambda)/dx) = 0, \qquad x = x_0, \tag{3e}$$

$$\alpha_n \psi_n(x, \lambda) + \beta_n p_n(d\psi_n(x, \lambda)/dx) = 0, \qquad x = x_n. \tag{3f}$$

Thus the original problem, Eqs. (1a)–(1c) has been replaced by the approximation, Eqs. (3a)–(3f). The computed eigenvalues Λ of the latter problem will be considered in what follows as approximations to the eigenvalues λ of problem (1a)–(1c). Moreover, the finer the resolution of the original interval of integration, the better an approximation of the eigenvalues of the original problem (Eqs. (1a)–(1c)) will be obtained, as was shown by our numerical experiments and in [14, 15].

The solution of Eq. (3a) for $\omega_k^2 > 0$ is

$$\psi_k(x, \lambda) = \psi_k(x_{k-1}, \lambda) \frac{\sin(\omega_k(x_k - x))}{\sin(\omega_k l_k)} + \psi_k(x_k, \lambda) \frac{\sin(\omega_k(x - x_{k-1}))}{\sin(\omega_k l_k)}, \tag{4a}$$

where $x_{k-1} < x < x_k$, $\omega_k l_k \neq j\pi$, $j = 1, 2, \ldots$. If $\omega_k^2 = 0$, then Eq. (4a) takes the form

$$\psi_k(x, \lambda) = \psi_k(x_{k-1}, \lambda)((x_k - x)/l_k) + \psi_k(x_k, \lambda)((x - x_{k-1})/l_k) \tag{4b}$$

If $\omega_k^2 < 0$, Eq. (4a) takes the form

$$\psi_k(x, \lambda) = \psi_k(x_{k-1}, \lambda) \frac{\sinh(\omega_k^*(x_k - x))}{\sinh(\omega_k^* l_k)} + \psi_k(x_k, \lambda) \frac{\sinh(\omega_k^*(x - x_{k-1}))}{\sinh(\omega_k^* l_k)}, \tag{4c}$$

$$\omega_k^* = (\mathrm{abs}(\omega_k^2))^{1/2}, \qquad k = 1, 2, \ldots, n. \tag{4d}$$

In Eqs. (4a)–(4c) the integration constants were expressed by means of the values of the eigenfunction at the endpoints of the corresponding subintervals.

To satisfy the external and interface boundary conditions of Eqs. (3c)–(3f), one has

$$((\alpha_0/\beta_0) + A_1)\, \psi_0(\lambda) - B_1 \psi_1(\lambda) = 0, \tag{5a}$$

$$-B_k \psi_{k-1}(\lambda) + (A_k + A_{k+1})\, \psi_k(\lambda) - B_{k+1} \psi_{k+1}(\lambda) = 0, \qquad k = 1, 2, \ldots, n-1, \tag{5b}$$

$$-B_n \psi_{n-1}(\lambda) + (A_n + (\alpha_n/\beta_n))\, \psi_n(\lambda) = 0, \tag{5c}$$

where

$$\psi_k(\lambda) = \psi_k(x_k, \lambda) = \psi_{k+1}(x_k, \lambda), \qquad k = 1, 2, \ldots, n-1, \tag{5d}$$

and

$$B_k = p_k\omega_k/\sin(\omega_k l_k), \qquad A_k = B_k\cos(\omega_k l_k), \qquad \omega_k^2 > 0, \tag{6a}$$

$$B_k = p_k/l_k, \qquad A_k = B_k, \qquad \omega_k^2 = 0, \tag{6b}$$

$$B_k = p_k\omega_k^*/\sinh(\omega_k^* l_k), \qquad A_k = B_k\cosh(\omega_k^* l_k), \qquad \omega_k^2 < 0, \tag{6c}$$

and $k = 1, 2, \ldots, n$.

Equations (5a)–(5c) form a linear system of $(n+1)$ homogeneous equations for the determination of $\psi_k(\lambda)$, $k = 0, 1, 2, \ldots, n$. In matrix notation it has the form

$$[K(\lambda)]\{\psi(\lambda)\} = 0, \tag{7a}$$

where

$$[K(\lambda)] = \begin{bmatrix} \bar{A}_1 & -B_1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ -B_1 & \bar{A}_1 & -B_2 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -B_2 & \bar{A}_2 & -B_3 & \cdots & 0 & 0 & 0 \\ \vdots & & \vdots & \vdots & & \vdots & & \vdots \\ 0 & \cdots & -B_{k-1} & \bar{A}_{k-1} & & -B_k & \cdots & 0 \\ \vdots & \cdots & & & & & \cdots & \vdots \\ 0 & \cdots & & 0 & & -B_{n-1} & \bar{A}_{n-1} & -B_n \\ 0 & \cdots & & 0 & & 0 & -B_n & \bar{A}_n \end{bmatrix}, \tag{7b}$$

$$\bar{A}_0 = (\alpha_0/\beta_0) + A_1, \tag{7c}$$

$$\bar{A}_k = A_{k-1} + A_k, \qquad k = 1, 2, 3, \ldots, n-1 \tag{7d}$$

$$\bar{A}_n = A_n + (\alpha_n/\beta_n), \tag{7e}$$

and

$$\{\psi(\lambda)\}^{\mathrm{T}} = \{\psi_0(\lambda), \psi_1(\lambda), \ldots, \psi_n(\lambda)\} \tag{7f}$$

is the transpose of $\{\psi(\lambda)\}$. In order that a nonzero solution for $\{\psi(\lambda)\}$ exists, one has

$$\det([K(\lambda)] = 0. \tag{8}$$

The infinite number of real roots of transcendental equation (8) are the eigenvalues of the approximate problem of Eqs. (3a)–(3f). Their computation is the core of the procedure to be described in the sections to follow.

3. Procedure for the Computation of the Eigenvalues

Wittrick and Williams [3, 4] developed an efficient procedure to compute the eigenfrequencies and the buckling loads of elastic linear skeletal structures. Since Eq. (8) is presented in the same form as that utilized by Wittrick and Williams, it is not difficult to adapt their procedure to the problem considered in the present paper.

Williams and Wittrick have shown that the number of positive eigenvalues $N(\tilde{\lambda})$ lying between zero and some prescribed positive value of $\lambda = \tilde{\lambda}$ is

$$N(\tilde{\lambda}) = N_0(\tilde{\lambda}) + s(|K(\tilde{\lambda})|, \tag{9}$$

where $N_0(\tilde{\lambda})$ is the number of positive eigenvalues not exceeding $\tilde{\lambda}$ when all components of the vector $\{\psi(\tilde{\lambda})\}$ corresponding to $|K(\tilde{\lambda})|$ are zero and $s(|K(\tilde{\lambda})|)$ denotes the "sign count" of $[K(\tilde{\lambda})]$.

To find $N_0(\tilde{\lambda})$ one takes into account the fact that since all components of the vector $\{\psi(\tilde{\lambda})\}$ are zero, the system of equations (3a) degenerates into a decoupled set of equations

$$(d^2\psi_k(x, \tilde{\lambda})/dx^2) + \tilde{\omega}_k^2 \psi_k(x, \tilde{\lambda}) = 0, \qquad x_{k-1} < x < x_k, \ k = 1, 2, \ldots, n, \tag{10a}$$

subject to the boundary conditions

$$\psi_k(x_{k-1}, \tilde{\lambda}) = 0, \tag{10b}$$

$$\psi_k(x_k, \tilde{\lambda}) = 0. \tag{10c}$$

The eigencondition of problem (10a)–(10c) is

$$\sin(\tilde{\omega}_k l_k) = 0. \tag{11a}$$

It has an explicit solution only if $\tilde{\omega}_k^2 > 0$, namely,

$$\tilde{\omega}_k l_k = j\pi, \qquad j = 1, 2, \ldots. \tag{11b}$$

Thus, $N_0(\tilde{\lambda})$ is equal to the total number of eigenvalues of the kind (Eq. (11b))

$$N_0(\tilde{\lambda}) = \sum_{k=1}^{n} \text{int}\left(\frac{\tilde{\omega}_k l_k}{\pi}\right), \tag{12}$$

where the value of the function int$(\cdot)$ is the largest integer not exceeding the value of the argument of the function.

The "sign count" is shown [3] to be equal to the number of negative elements along the main diagonal of the matrix $[K^{\Delta}(\tilde{\lambda})]$, which is the triangulated form of the matrix $[K(\tilde{\lambda})]$, or equivalently, the number of negative elements in the sequence

D_1/D_0, D_2/D_1, D_3/D_2,..., D_n/D_{n-1}, where D_k, $k = 1, 2,..., n$, denotes the kth order principal minor of the matrix $[K(\tilde{\lambda})]$, $D_0 = 1$, $D_1 = \bar{A}_1$. In view of the tridiagonal structure of this matrix, one has

$$D_k = D_{k-1}(A_k + A_{k-1}) - D_{k-2}B_{k-1}^2, \qquad k = 2, 3,..., n. \tag{13}$$

The case of Dirichlet boundary conditions at $x = x_0$ or at $x = x_n$ or at both endpoints corresponds to $\beta_0 = 0$ or/and $\beta_n = 0$, thus resulting in $\bar{A}_1 \to \infty$ or/and $\bar{A}_n \to \infty$. In any of these case one simply neglects the corresponding row and column of $[K(\tilde{\lambda})]$ as they do not influence the elimination process described by Eq. (13) and imply $\psi_1(x_0, \tilde{\lambda}) = 0$ or/and $\psi_n(x_n, \tilde{\lambda}) = 0$.

As both terms on the right-hand side of Eq. (9) can be computed, one has the following algorithm to calculate any positive eigenvalue of the approximate problem of Eqs. (3a)–(3f):

Step 1. Prescribe values of i, the order of the eigenvalue λ_i desired and ε_i, the (absolute) accuracy in λ_i; set lower bound for λ_i, $\lambda_l = 0$, upper bound for λ_i, $\lambda_u = 0$, current value of the λ-parameter, $\lambda = 0$; in case there is additional information concerning λ_i, set more appropriate values for the parameters listed to save computer time.

Step 2. Define the increment δ in $\tilde{\lambda}$, $\delta \neq 0$; set $\tilde{\lambda} = \tilde{\lambda} + \delta$, $\lambda_u = \tilde{\lambda}$; compute $N(\tilde{\lambda})$.

Step 3. If $N(\tilde{\lambda}) \geqslant i$, go to Step 5, else go to Step 4.

Step 4. Parameter $\tilde{\lambda}$ is a lower bound for λ_i; set $\lambda_l = \tilde{\lambda}$, go to Step 2.

Step 5. Parameter $\tilde{\lambda}$ is an upper bound for λ_i; set $\lambda_u = \tilde{\lambda}$.

Step 6. Compute $\Delta\lambda = \text{abs}(\lambda_u - \lambda_l)$; if $\Delta\lambda \leqslant \varepsilon_i$, go to Step 10, else go to Step 7.

Step 7. Compute $\tilde{\lambda} = (\lambda_u + \lambda_l)/2$; compute $N(\tilde{\lambda})$.

Step 8. If $N(\tilde{\lambda}) \geqslant i$, set $\lambda_u = \tilde{\lambda}$ and go to Step 6, else go to Step 9.

Step 9. Set $\lambda_l = \tilde{\lambda}$; go to Step 6.

Step 10. $\lambda_i = (\lambda_u + \lambda_l)/2$.

4. Computation of the Eigenfunctions

Once the eigenvalue λ_i has been located, one might want to know some values of the eigenfunction $\psi_i(x, \lambda_i)$ at (possibly) previously prescribed positions. The computation of the eigenfunction can be carried out making use of Eqs. (5) and (6). The choice of $\psi_{i,1}(x_0, \lambda_i) = \beta_0$ and $p_1(d/dx)\,\psi_{i,1}(x_0, \lambda_i) = \alpha_0$ satisfies identically Eq. (3e). Therefore, introducing

$$\psi_{i,0}(\lambda_i) = \beta_0 \tag{14a}$$

into Eq. (5a), one obtains

$$\psi_{i,1}(\lambda_i) = (\alpha_0 + A_1\beta_0)/B_1. \tag{14b}$$

Equation (5b) can be rewritten as

$$\psi_{i,k+1}(\lambda_i) = ((A_k + A_{k+1})\,\psi_{i,k}(\lambda_i) - B_k\psi_{k-1}(\lambda_i))/B_{k+1}, \qquad k = 1, 2,..., n-1. \tag{14c}$$

The last recurrence relation, Eq. (14c), enables one to compute all the components of the vector $\{\psi(\lambda_i)\}$ of Eq. (7f), which are the values of the eigenfunction $\psi_i(x, \lambda_i)$ corresponding to the eigenvalue λ_i at the endpoints of the subintervals l_k, $k = 1, 2,..., n$.

From Eqs. (5) it can be seen that in case the exact eigenvalues of the approximate problem (Eqs. (3)) are known and if the coefficients A_k and B_k, $k = 1, 2,..., n$, of Eqs. (6) can be computed exactly, then Eq. (5c) should be satisfied identically. But to the extent that the computation cannot be performed exactly and the eigenvalues can be computed approximately in the sense of the algorithm described in Section 3, the left-hand side of Eq. (5c) cannot become zero. Its value can be considered as an estimate for the global error in the computation of the eigenfunction. For the special case of a Dirichlet boundary, when Eq. (5c) is not considered, the accuracy estimate can be obtained by Eq. (5b), written for $k = n - 1$ and bearing in mind that that $\psi_{i,n}(\lambda_i) = 0$.

The norm $\mathcal{N}_i$ of the eigenfunction $\psi_i(x, \lambda_i)$ can be defined as

$$\mathcal{N}_i^2 = \sum_{k=1}^{n} r_k \int_{x_{k-1}}^{x_k} \psi_{i,k}^2(x, \lambda_i)\, dx, \tag{15}$$

and in view of Eqs. (4) and (6) one has

$$\int_{x_{k-1}}^{x_k} \psi_{i,u}^2(x, \lambda_i)\, dx = (2p_k\omega_k^2)^{-1}\{(\psi_{k-1}^2 + \psi_k^2)(B_k^2 l_k/p_k - A_k) + 2B_k\psi_{k-1}\psi_k(1 - A_k l_k/p_k)\}, \tag{16}$$

where $\psi_k = \psi_{i,k}(x_k, \lambda_i)$ and the constant ω_k^2, A_k, and B_k are calculated for $\lambda = \lambda_i$.

5. Choosing Step Sizes

The purpose of the procedure to be described is to construct the division of the interval $[a, b]$ into subintervals l_k, $k = 1, 2,..., n$, in such a manner that the local error in the values of the eigenfunction computed be held at a prescribed level and be of comparable magnitude for any of the subintervals necessary to approximate the original problem.

Our strategy is based on the assumption that the eigenfunction is quite sensitive in respect to the eigenvalue parameter λ. Thus, if one is able to compute the values of

some function $\bar{\psi}_i(x, \bar{\lambda}_i)$ that oscillates at least as rapidly as the eigenfunction wanted, where $\bar{\lambda}_i$ is some upper bound for the eigenvalue λ_i, on the basis of two different divisions of the interval $[a, b]$, the second of them j times finer than the first, and the corresponding values computed are equal in the sense of some predetermined local error level, then the rougher of these two divisions of $[a, b]$ could be used to compute the desired eigenvalue and the corresponding eigenfunction with approximately the same local accuracy.

Having in mind the procedure described in the previous section for the computation of the eigenfunction, the following principal algorithm could be used to find the division of $[a, b]$:

Step 1. Prescribe the following quantities: upper and lower bounds $\varepsilon_{\max}$ and $\varepsilon_{\min}$, respectively, for the local error of the function $\bar{\psi}_i(x, \bar{\lambda}_i)$ for an arbitrary subinterval, where i is the order of the eigenvalue λ_i and the corresponding eigenfunction $\psi_i(x, \lambda_i)$ to be computed; $\bar{\lambda}_i$ is an upper bound of λ_i and $\bar{\psi}_i(x, \bar{\lambda}_i)$ oscillates at least as rapidly as $\psi_i(x, \lambda_i)$; l_0 is the initial guess for the first subinterval $l_1 = x_1 - x_0$; $l_{\min}$ is the minimal admissible length of an arbitrary subinterval of the division of $[a, b]$ to be computed (the maximum admissible length for the subinterval is $[a, b]$ itself); fix an integer j by means of which a j times finer division of $[a, b]$ could be generated.

Step 2. Set $k = 1$, $l = l_0$, $\bar{x} = x_0$.

Step 3. Set $l_j = l/j$.

Step 4. Compute $\bar{\psi}_i(\bar{x} + l, \bar{\lambda}_i)$ directly from Eqs. (14).

Step 5. Compute $\bar{\psi}_i^{(j)}(\bar{x} + l, \bar{\lambda}_i)$, utilizing successively the values $\bar{\psi}_i(\bar{x} + l_j, \bar{\lambda}_i)$, $\bar{\psi}_i(\bar{x} + 2l_j, \bar{\lambda}_i)$,..., $\bar{\psi}_i(\bar{x} + (j-1)l_j, \bar{\lambda}_i)$, and Eqs. (14).

Step 6. If $\bar{\psi}_i^{(j)}(\bar{x} + l, \bar{\lambda}_i)$ and $\bar{\psi}_i(\bar{x} + l, \bar{\lambda}_i)$ are equal in the sense of the local error prescribed, go to Step 9; else go to Step 7.

Step 7. If $l < l_{\min}$, go to Step 12; else go to Step 8.

Step 8. Decrease (set $l = l_j$) or increase (set $l = jl$) the guess for the subinterval considered and go to Step 3.

Step 9. Accuracy requirements are satisfied; set $l_k = l$, $\bar{x} = \bar{x} + l$, $k = k + 1$.

Step 10. If $\bar{x} + l = x_n$, go to Step 3; else go to Step 11.

Step 11. This is the correct exit of the algorithm; the last subinterval has to be adjusted so that $l_n = x_n - \bar{x}$ in the sense of some error tolerance. At this place one has the number of the subintervals for the eigenvalue considered $n = k + 1$ and the division of $[a, b]$ into n subintervals, thus being able to utilize the algorithms for the computation of λ_i and $\psi_i(x, \lambda_i)$ described earlier.

Step 12. This is the error exit, indicating in general that the accuracy requirements are not appropriately chosen.

The estimate $\bar{\lambda}_{i+1}$ for the next eigenvalue λ_{i+1} can be obtained utilizing the division by means of which λ_i and $\psi_i(x, \lambda_i)$ have been computed and $\bar{\lambda}_1$ can be obtained starting from some initial (e.g., uniform) division of $[a, b]$.

A simpler approach can be used by finding an estimate $\bar{\lambda}_m$ for the eigenvalue λ_m, where m is the order of the highest eigenvalue that has to be computed.

A check on the global error of the ψ function computed can be performed by making use of Eq. (5c) or Eq. (5b) for $k = n - 1$ as was described in the previous section; thus the inequality should be satisfied

$$\text{abs}(-B_n \bar{\psi}_i(x_{n-1}, \bar{\lambda}_i) + \bar{A}_n \bar{\psi}_i(x_n, \bar{\lambda}_i)) \leqslant \varepsilon_{\text{global}}, \tag{17}$$

where for an upper bound for the global error one can assume

$$\varepsilon_{\text{global}} \simeq \varepsilon_{\max} \cdot n. \tag{18}$$

In case Eq. (5b) has to be used instead of Eq. (5c), one sets $k = n - 1$ and obtains the corresponding expression for the left-hand side of Eq. (17).

The choice of step sizes in our method, as seen from the above, is not directly related to the eigenvalue under consideration, since the analytical function representing the eigenfunction may have any number of oscillations in a single subinterval.

6. Applicability of the Algorithm

To discuss the applicability of this algorithm one has to recall some well-known qualitative results from the theory of the one-dimensional linear Sturm–Liouville problems. Ince has shown [17, Sect. 10.61] that if $p(x) > 0$, $r(x) > 0$, and $q(x) \geqslant 0$ in the finite interval $[a, b]$, and if these three functions together with the coefficients α_0, β_0, α_n, and β_n do not depend on the eigenvalue parameter λ, then the corresponding regular eigenvalue problem has a numerable set of positive eigenvalues

$$0 < \lambda_1 < \lambda_2 < \cdots \tag{19}$$

with $+\infty$ as the only limit point of the sequence in Eq. (19). This is the case discussed in the previous sections.

If $q(x)$ changes sign in $[a, b]$, the set of the eigenvalues has the same character with the only exception that the sequence in Eq. (19) is shifted towards the negative semiaxis and $\lambda_1 \geqslant \min(q(x))$, $a \leqslant x \leqslant b$. So let

$$\lambda = \mu - C, \qquad \Lambda = M - C, \tag{20a}$$

and substitute Eq. (20a) into Eq. (1a) to obtain

$$(d/dx)(p(x)(d\Psi(x, M)/dx) + (Mr(x) - q^*(x))\,\Psi(x, M) = 0, \tag{20b}$$

where

$$q^*(x) = Cr(x) + q(x) \tag{20c}$$

and the constant C is chosen so that $q^*(x) \geqslant 0$, $a \leqslant x \leqslant b$. The shifted problem of Eq. (20b) can readily be solved utilizing the algorithm described to find a sequence of eigenvalues

$$0 < \mu_1 < \mu_2 < \cdots \tag{20d}$$

and through Eq. (20a) to recover the original spectrum λ_i, $i = 1, 2, \ldots$.

Ince has also shown that if $r(x)$ changes sign in $[a, b]$ while $q(x) \geqslant 0$ there, then one has for the spectrum

$$-\infty < \cdots < \lambda_n^- < \lambda_{n-1}^- < \cdots < \lambda_1^- < 0 < \lambda_1^+ < \lambda_2^+ < \cdots < +\infty. \tag{21a}$$

After computing the positive part of the spectrum as was already described, one might set

$$\lambda = -\nu, \tag{21b}$$

which is equivalent to a reversal of the sign of $r(x)$; in this way one is able to compute the negative part of the spectrum to such a problem.

The next case to be considered is the presence of interface resistance $h_{k,k+1}$ [18, 19] between two subintervals l_k and l_{k+1} of the division of $[a, b]$. Now, boundary condition (3d) takes the form

$$p_k(d\psi_k(x_k, \lambda)/dx) = h_{k,k+1}(\psi_{k+1}(x_k, \lambda) - \psi_k(x_k, \lambda)). \tag{22a}$$

Assume that one could insert a fictitious subinterval $l_{k,k+1}$ between the subintervals l_k and l_{k+1}, such that $\omega_{k,k+1}^2 = 0$. Consequently, $r_{k,k+1} = 0$ and $q_{k,k+1} = 0$. Taking arbitrary values for $p_{k,k+1}$ and $l_{k,k+1}$ such that

$$p_{k,l+1}/l_{k,k+1} = h_{k,k+1}, \tag{22b}$$

the procedure described above can again be applied to solve the corresponding Sturm–Liouville eigenproblem.

The last class of problems to be considered in this section is that of the singular problems, characterized by infinite endpoint singularities. The theory developed in [20, Part 1, Chap. V, 5.1] considers the complex Sturm–Liouville problem and states that (only case $b \to \infty$ will be considered):

(i) if $b \to \infty$ and $\lim_{x \to b} q(x) = \infty$, the spectrum is numerable;

(ii) if $b \to \infty$ and $\lim_{x \to b} q(x) = q_0$, where q_0 is finite, then the spectrum has either a finite discrete component and a continuous component or it is continuous;

(iii) if $b \to \infty$ and $\lim_{x \to b} q(x) = -\infty$ while the integral

$$\int_a^{\infty} \operatorname{abs}(q(x))^{-1/2}\, dx$$

has a finite limit (a is assumed to be finite), one has the spectrum of (i); otherwise the spectrum is continuous.

Case (iii) will not be considered in what follows inasmuch as the authors have no evidence of the applicability of this case to real Sturm–Liouville problems.

To discuss cases (i) and (ii), first recall Eq. (6c). The constants A_k and B_k can be rewritten as

$$A_k = p_k \omega_k^* (1 + \exp(-2\omega_k^* l_k))(1 - \exp(2\omega_k^* l_k))^{-1}, \tag{23a}$$

$$B_k = 2A_k \exp(-\omega_k^* l_k)(1 + \exp(-2\omega_k^* l_k))^{-1}, \tag{23b}$$

and one recalls that $\omega_k^2 < 0$. Usually, when one solves numerically some initial or boundary value problem defined on an infinite interval, he either explicitly or implicitly assumes that the solution changes significantly over some reasonable long finite subinterval, while over the remaining infinite subinterval the solution is assumed to have some asymptotic behavior. This implies that for the singular problems under consideration one has to separate the infinite interval $[a, \infty)$ into a finite subinterval $[a, c]$ and an infinite subinterval (c, ∞). Over the former of these one can apply the procedure developed in the previous sections, while in this section the infinite subinterval (c, ∞) will be paid some particular attention. It is seen from Eqs. (23) that $l_k \to \infty$ implies $B_k \to 0$ and $A_k \to p_k \omega_k^* \geqslant 0$.

For case (i), $q(x) \to \infty$ implies $A_k \to \infty$ and $B_k \to 0$ independently of l_k. Consequently, the finite subinterval $[a, c]$ can be fixed from the condition that B_k behaves as zero in the sense of the machine word length. Having in mind the fact that $A_k \to \infty$, the last two rows and columns of the matrix $|K(\lambda)|$, which correspond to the infinite interval (c, ∞), are eliminated from consideration, similarly to the ones used for Dirichlet boundary conditions at a finite endpoint of a regular problem. Consequently, for case (i) one can apply the algorithm already discussed. Our conclusion corresponds to Bailey *et al.* [2] in the sense that for a limit point singularity the solution approaches the singular point regardless of the boundary condition imposed there.

Case (ii) can be treated in a similar manner. Now $B_k \to 0$, but A_k remains finite. Thus, the finite subinterval $[a, c]$ has to be determined from the condition that A_k behaves as a constant as $x \to b$ and the corresponding subintervals remain finite. After this has been done, one fixes the division of $[a, \infty)$ as composed of a finite number of finite subintervals plus the infinite subinterval (c, ∞). This means that if the division of $[a, c]$ comprises n subintervals, the division of $[a, \infty)$ will comprise $n + 1$ subintervals, the last of which will be the infinite one. Consequently, $\bar{A}_{n+1}$ will have the form

$$\bar{A}_{n+1} = p_{n+1} \omega_{n+1}^* + (\alpha_n / \beta_n), \tag{24}$$

having in mind that for the case under consideration $p(x) = 1$. This formulation corresponds to [12] in the sense that when a limit circle singularity is present, the solution advances towards the singular endpoint following a trajectory prescribed by the particular boundary condition imposed at the singular endpoint. Moreover, as Eqs. (23) are valid for $\omega_k^2 < 0$, it is clear that if $q_0 < 0$ (depending on $r(x)$, which is supposed bounded and nonnegative), one may have a finite number of eigenvalues on the negative semiaxis, while otherwise the whole spectrum will be continuous.

7. Test Calculations

The procedure for the computation of the eigenvalues and the eigenfunctions developed in this paper was programmed in APPLESOFT BASIC and a number of test examples were calculated on an APPLE II personal computer. The code was tested on a number of problems, the solutions of which had been previously published. Some illustrative results are presented in Table I. The symbols appearing in column 1 of this table are the same as in the original references.

First, regular problems with constant coefficients subject to different boundary conditions [21] were solved. The eigenvalues of each particular problem were calculated utilizing several different divisions of the integration interval into subintervals. The results for the eigenvalues of a particular problem obtained through the various divisions were fully coincident—row 1 from Table I. Next, some discontinuous coefficient problems on finite intervals were solved [22, 23], utilizing the same testing strategy—row 2 in Table I. Our results are in full agreement with the corresponding references.

We resolved most of the problems from [14, 15]. No case of missing eigenvalues was identified. This test also proved the applicability of our algorithm for practically asymptotic problems. Some illustrative results are given in row 3 of Table I.

TABLE I

Problem	λ_1	λ_2	λ_3
Mikhailov [1] $Bi_0 = 1, Bi_1 = 1$	1.7070	13.4923	43.3572
Muhlholland and Cobbler [23]	277.433	1953.73	3404.21
Canosa and de Oliveira [14] $q = 1600, n = 104$ Neumann boundary	−3119.20	−2959.43	−2801.85
Nunge and Gill [24] $N = 1.73, n = 100$	5.9801 −0.00	304.453 −80.8314	997.897 −263.279

The last test to be discussed here is the recalculation of the first three eigenvalues $\lambda_i^+ c$ and λ_i^-, $i = 1, 2, 3$ from [24]—row 4 of Table I. Again there is full agreement between our results and the ones obtained in the original reference.

The test calculations for infinite endpoint singular Sturm–Liouville problems as discussed in the previous section are presently in preparation. The tests performed to verify the procedure for the computation of the eigenfunctions and the choice of step sizes gave more than encouraging results. They will be discussed in a future publication together with some algorithmic and programming details concerning the code.

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