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Spectral corrections for Sturm–Liouville problems ☆

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Abstract

The numerical solution of the Sturm–Liouville problem can be achieved using shooting to obtain an eigenvalue approximation as a solution of a suitable nonlinear equation and then computing the corresponding eigenfunction. In this paper we use the shooting method both for eigenvalues and eigenfunctions. In integrating the corresponding initial value problems we resort to the boundary value method. The technique proposed seems to be well suited to supplying a general formula for the global discretization error of the eigenfunctions depending on the discretization errors arising from the numerical integration of the initial value problems. A technique to estimate the eigenvalue errors is also suggested, and seems to be particularly effective for the higher-index eigenvalues. Numerical experiments on some classical Sturm–Liouville problems are presented. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

We consider the regular Sturm–Liouville problem (SLP)

$$-(p(x)u')' + q(x)u = \lambda w(x)u, \quad -\infty < a \leqslant x \leqslant b < +\infty, \tag{1}$$

$$a_1 u(a) - a_2 p(a)u'(a) = 0, \tag{2}$$

$$b_1 u(b) - b_2 p(b)u'(b) = 0, \tag{3}$$

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where $p, q, w \in C^{\omega}$, for some integer ω, on the interval $[a, b]$, with $p(x) > 0$, $w(x) > 0$, and where a_1, a_2 are real with $|a_1| + |a_2| \neq 0$ and similarly for b_1 and b_2.

For convenience we introduce the following notations:

$$H(x,\lambda) = \begin{pmatrix} 0 & 1/p \\ q - \lambda w & 0 \end{pmatrix}, \quad z(x) = \begin{pmatrix} u \\ pu' \end{pmatrix},$$
$$A = \begin{pmatrix} a_1 & -a_2 \\ 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 \\ b_1 & -b_2 \end{pmatrix}.$$

Thus the SLP (1)–(3) can be written in the form (see [15, Chapter 1])

$$z' = H(x,\lambda)z, \tag{4}$$

$$Az(a) + Bz(b) = 0, \tag{5}$$

where $\operatorname{rank}(A, B) = 2$.

The aim of the present paper is to compute a numerical approximation of an eigenvalue λ of problem (4)–(5) and the associated eigenfunction $z(x)$ as well as the corresponding discretization error which can be used as correcting term. The shooting method will be employed ([8, Chapter 4; 18, Chapter 5]) in combination with the boundary value method (BVM) as discretization method [9]. There are several papers concerning the computation and the correction of the eigenvalues (see, for example, [2–7,10,16,17,19–23]). In the case of the correction of the eigenfunctions see, for example, [13,14,18, Chapter 9], with references therein.

In the next section we establish a general method for estimating the global discretization error (GDE) in the numerical computation of an eigenfunction; the technique is based upon an idea given in [11].

Let $\{a = \tau_0 < \tau_1 < \cdots < \tau_m = b\}$ be a partition of the interval $[a, b]$ and let $W_j(x) \in \mathbb{R}^{2\times 2}$, $j = 1, 2, \ldots, m$, be the fundamental matrix solutions of the initial value problems (IVPs)

$$\begin{aligned} &W_j'(x) = H(x,\lambda)W_j(x), \quad \tau_{j-1} \leqslant x \leqslant \tau_j, \\ &W_j(\tau_{j-1}) = I, \quad j = 1, 2, \ldots, m, \end{aligned} \tag{6}$$

with I the identity matrix.

For a given λ the solution of (4)–(5) is

$$z(x) \equiv z_j(x) = W_j(x)s_j, \quad j = 1, 2, \ldots, m,$$

where the vectors $s_1, s_2, \ldots, s_m$ are chosen in order to ensure the continuity of $z(x)$ across the interior shooting nodes τ_j, $j = 1, 2, \ldots, m-1$, and to satisfy the boundary conditions (5). These requirements lead to the system

$$\begin{aligned} &W_1(\tau_1)s_1 - s_2 = 0 \\ &W_2(\tau_2)s_2 - s_3 = 0 \\ &\vdots \\ &W_{m-1}(\tau_{m-1})s_{m-1} - s_m = 0 \\ &As_1 + BW_m(\tau_m)s_m = 0, \end{aligned} \tag{7}$$

from which we have

$$\begin{aligned} s_2 &= W_1(\tau_1)s_1 \\ s_3 &= W_2(\tau_2)W_1(\tau_1)s_1 \\ &\vdots \\ s_m &= W_{m-1}(\tau_{m-1})\cdots W_1(\tau_1)s_1 \\ [A + BW_m(\tau_m)\cdots W_1(\tau_1)]s_1 &= 0. \end{aligned} \tag{8}$$

The fundamental matrices depend on λ so that system (7) has a nontrivial solution $s=(s_1^{\mathrm{T}}, s_2^{\mathrm{T}}, \ldots s_m^{\mathrm{T}})^{\mathrm{T}}$ if the values of λ are the eigenvalues of problem (4)–(5), i.e. the solutions of the nonlinear scalar equation

$$\det[A + BW_m(\tau_m)\cdots W_1(\tau_1)] = 0.$$

From the last equation in (8) we verify that for any eigenvalue the corresponding eigenfunction can be obtained assuming $s_1 = (a_2, a_1)^{\mathrm{T}}$ and then solving the linear system

$$Ms^* = c, \tag{9}$$

where $s^* = (s_2^{\mathrm{T}}, s_3^{\mathrm{T}}, \ldots, s_m^{\mathrm{T}})^{\mathrm{T}}$ and

$$M = \begin{pmatrix} -I & & & \\ W_2(\tau_2) & -I & & \\ & \ddots & \ddots & \\ & & W_{m-1}(\tau_{m-1}) & -I \end{pmatrix}, \quad c = \begin{pmatrix} -W_1(\tau_1)s_1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

While the solution of system (9) could be computed, in some instances, by recursion (8), this process is generally unstable, being similar to Gaussian elimination without partial pivoting. This is particularly true in the many cases where multiple shooting is essential to obtain accurate answers. The formulation (9) is therefore to be preferred.

2. GDE for eigenfunctions

In practice the exact value of an eigenvalue λ is not available, but rather an approximation μ. Thus the IVPs to be solved are

$$\begin{aligned} V_j'(x) &= H(x,\mu)V_j(x), \quad \tau_{j-1} \leqslant x \leqslant \tau_j, \\ V_j(\tau_{j-1}) &= I, \quad j = 1,2,\ldots,m, \end{aligned} \tag{10}$$

instead of (6).

We consider the mesh points $x_i = x_0 + ih$, $i = 0,1,\ldots,n$, with constant steplength $h=(b-a)/n$ and $n=ml$ for some integer l. Therefore the shooting nodes are $\tau_0 = x_0, \tau_1 = x_l, \ldots, \tau_{m-1} = x_{(m-1)l}, \tau_m = x_n$.

We use a numerical method of order p to integrate (10) obtaining the approximations V_{ji} to $V_j(x_i)$, namely $V_j(x_i) = V_{ji} + \mathrm{O}(h^p)$, and an approximation $\sigma = (\sigma_1^{\mathrm{T}}, \sigma_2^{\mathrm{T}}, \ldots, \sigma_m^{\mathrm{T}})^{\mathrm{T}}$ to s.

In fact, we have to solve the system

$$N\sigma^* = d, \tag{11}$$

where $\sigma^* = (\sigma_2^{\mathrm{T}}, \sigma_3^{\mathrm{T}}, \ldots, \sigma_m^{\mathrm{T}})^{\mathrm{T}}$ and

$$N = \begin{pmatrix} -I & & & \\ V_{2,2l} & -I & & \\ & \ddots & \ddots & \\ & & V_{m-1,(m-1)l} & -I \end{pmatrix}, \quad d = \begin{pmatrix} -V_{1l}s_1 \\ 0 \\ \vdots \\ 0 \end{pmatrix},$$

instead of (9), provided that μ is now a solution of the scalar equation

$$f(\mu, h) = 0, \tag{12}$$

where $f(\mu, h) = \det[A + BV_{m,ml} \cdots V_{1l}]$, and assuming $\sigma_1 = s_1$. Thus μ and $V_j(x)$ depend on h.

The following lemma holds.

Lemma 2.1. *If*

$$\lambda - \mu = \mathrm{O}(h^q)$$

for some real $q > 0$, *then*

$$W_j(x_i) - V_j(x_i) = \mathrm{O}(h^q), \quad j = 1, 2, \ldots, m, \ i = (j-1)l, \ldots, jl.$$

Proof. By subtracting (10) from (6) we obtain the IVPs

$$\begin{aligned} &D_j'(x) = H(x, \lambda)D_j(x) + (\lambda - \mu)Q_j(x), \quad \tau_{j-1} \leqslant x \leqslant \tau_j, \\ &D_j(\tau_{j-1}) = 0, \quad j = 1, 2, \ldots, m, \end{aligned} \tag{13}$$

with $D_j(x) = W_j(x) - V_j(x)$ and

$$Q_j(x) = \begin{pmatrix} 0 & 0 \\ -w(x) & 0 \end{pmatrix} V_j(x). \tag{14}$$

The proof follows observing that the solutions of (13) are given by

$$D_j(x) = (\lambda - \mu)W_j(x) \int_{\tau_{j-1}}^{x} W_j^{-1}(t)Q_j(t)\,\mathrm{d}t, \quad \tau_{j-1} \leqslant x \leqslant \tau_j, \ j = 1, 2, \ldots, m,$$

and $V_j(x)$ are not vanishing when $h \to 0$. □

We define the GDE for the eigenfunction $z(x)$ as

$$e_j(x_i) = z_j(x_i) - y_{ji}, \quad j = 1, 2, \ldots, m, \ i = (j-1)l, \ldots, jl,$$

where $z_j(x_i) = W_j(x_i)s_j$ and $y_{ji} = V_{ji}\sigma_j$.

Let

$$R_j(x_i) = V_j(x_i) - V_{ji}, \quad j = 1,2,\ldots,m,\ i = (j-1)l,\ldots,jl,$$

be the discretization errors arising from the integration of the IVPs (10).

Define the $(m-1)$-vector $r=(r_1^{\mathrm{T}}, r_2^{\mathrm{T}},\ldots,r_{m-1}^{\mathrm{T}})^{\mathrm{T}}$ with $r_j = R_j(\tau_j)\sigma_j$, $j=1,2,\ldots,m-1$. The following theorem holds.

Theorem 2.1. *Suppose that μ is a solution of Eq. (12) and an approximation to λ of order q. Then for the GDE associated with the eigenfunction $z(x)$ we have*

$$\begin{aligned}
e_1(x_i) &= R_1(x_i)s_1 + \mathrm{O}(h^q), \quad i = 0,1,\ldots,l,\\
e_2(x_i) &= V_2(x_i)r_1 + R_2(x_i)\sigma_2 + \mathrm{O}(h^q), \quad i = l, l+1,\ldots,2l,\\
e_j(x_i) &= V_j(x_i)\left\{\sum_{\gamma=1}^{j-2}\left[\prod_{k=0}^{j-\gamma-2} V_{j-k-1}(\tau_{j-k-1})\right] r_\gamma + r_{j-1}\right\}\\
&\quad + R_j(x_i)\sigma_j + \mathrm{O}(h^q), \quad j = 3,4,\ldots,m,\ i = (j-1)l,\ldots,jl.
\end{aligned} \tag{15}$$

Proof. We define a vector δ whose components are $\delta_j = s_j - \sigma_j$, $j = 2,3,\ldots,m$, and $\delta_1 = 0$. From Lemma 2.1, the GDE can now be written as

$$e_j(x_i) = V_j(x_i)\delta_j + R_j(x_i)\sigma_j + \mathrm{O}(h^q), \quad j = 1,2,\ldots,m,\ i = (j-1)l,\ldots,jl. \tag{16}$$

The $(m-1)$-vector $\delta^* = (\delta_2^{\mathrm{T}}, \delta_3^{\mathrm{T}},\ldots,\delta_m^{\mathrm{T}})^{\mathrm{T}}$ is the solution of the linear system

$$P\delta^* = -r + \mathrm{O}(h^q), \tag{17}$$

where

$$P = \begin{pmatrix} -I & & & \\ V_2(\tau_2) & -I & & \\ & \ddots & \ddots & \\ & & V_{m-1}(\tau_{m-1}) & -I \end{pmatrix}.$$

In fact, (17) results from subtracting (11) from (9) and adding to the jth equation the null term $V_j(\tau_j)\sigma_j - V_j(\tau_j)\sigma_j$, $j = 2,3,\ldots,m-1$.

The proof follows by direct forward substitution starting from the first equation of system (17). □

Remark 2.1. Recalling that $V_j(\tau_j) = V_{j,jl} + \mathrm{O}(h^p)$, $j=2,3,\ldots,m-1$, we have $P = N + \mathrm{O}(h^p)$. Therefore, by the perturbation lemma, it follows that $P^{-1} = N^{-1} + \mathrm{O}(h^p)$ too. Because $R_j(x_i)\sigma_j = \mathrm{O}(h^p)$, then

$\tilde{\delta}^* = -N^{-1}r$ is an approximation to δ^* for which $\delta^* = \tilde{\delta}^* + \mathrm{O}(h^{2p}) + \mathrm{O}(h^q)$. Setting $\tilde{\delta} = (0^{\mathrm{T}}, \tilde{\delta}^{*^{\mathrm{T}}})^{\mathrm{T}}$ and assuming $\tilde{e}_j(x_i) = V_{ji}\tilde{\delta}_j + R_j(x_i)\sigma_j$ as an estimation of the GDE, from (16) we have

$$e_j(x_i) = \tilde{e}_j(x_i) + \mathrm{O}(h^t),$$

where

$$t = \min\{2p, q\}.$$

3. Computing the discretization errors for IVPs

In formulas (15) we need to compute the discretization errors $R_j(x_i)$. An useful approach is to resort to a BVM (see [9, Chapter 4]) in integrating the IVPs (10). For the sake of the simplicity we consider the IVPs in the generic form

$$\begin{aligned} &U'(x) = H(x,\mu)U(x), \quad x_0 \leqslant x \leqslant x_\eta, \\ &U(x_0) = I, \end{aligned} \tag{18}$$

where $[x_0, x_\eta]$ is any of the m constant length shooting intervals previously defined, i.e. $x_0 = \tau_{j-1}$ and $x_\eta = \tau_j$, for some $j \in [1, m]$.

Let

$$\begin{aligned} &\sum_{i=0}^{k^*} \alpha_{iv} U_i = h \sum_{i=0}^{k^*} \beta_{iv} H(x_i, \mu) U_i, \quad v = 1, \ldots, k_1 - 1, \\ &\sum_{i=0}^{k} \alpha_i U_{v+i-k_1} = h \sum_{i=0}^{k} \beta_i H(x_{v+i-k_1}, \mu) U_{v+i-k_1}, \quad v = k_1, \ldots, \eta - k_2, \\ &\sum_{i=0}^{k^*} \alpha_{iv} U_{\eta+i-k^*} = h \sum_{i=0}^{k^*} \beta_{iv} H(x_{\eta+i-k^*}, \mu) U_{\eta+i-k^*}, \quad v = \eta - k_2 + 1, \ldots, \eta, \end{aligned} \tag{19}$$

be a pth-order BVM for (18) with (k_1, k_2) boundary conditions, where $k_1 + k_2 = k$, $k^* \leqslant k$ and with the linear multistep formulas fixed-h BVM stable.

The BVM (19) can be written in a more convenient form. In fact the matrix $U = (U_1^{\mathrm{T}}, U_2^{\mathrm{T}}, \ldots, U_\eta^{\mathrm{T}})^{\mathrm{T}}$ formed from the approximations U_i of the exact values $U(x_i)$, $i = 1, 2, \ldots, \eta$, can be computed as the solution of the linear system

$$GU = \Gamma, \tag{20}$$

where Γ contains the initial values and

$$G = G_\alpha \otimes I - h(G_\beta \otimes I)H. \tag{21}$$

In (21) $\otimes$ denotes the right Kronecker product, I the identity matrix of order 2, $H = \mathrm{diag}(H(x_1,\mu), H(x_2,\mu),\dots,H(x_\eta,\mu))$ and the $\eta\times\eta$ matrices G_α and G_β are given by

$$G_\alpha = \begin{pmatrix}
\alpha_{11} & \cdots & \alpha_{k^*1} & & & & & \\
\cdots & \cdots & \cdots & & & & & \\
\alpha_{1,k_1-1} & \cdots & \alpha_{k^*,k_1-1} & & & & & \\
\alpha_1 & \cdots & \cdots & \cdots & \alpha_k & & & \\
\alpha_0 & \cdots & \cdots & \cdots & \cdots & \alpha_k & & \\
 & \ddots & & & & & \ddots & \\
 & & \alpha_0 & \cdots & \cdots & \cdots & \cdots & \alpha_k \\
 & & & & \alpha_{0,\eta-k_2+1} & \cdots & \cdots & \alpha_{k^*,\eta-k_2+1} \\
 & & & & \cdots & \cdots & \cdots & \cdots \\
 & & & & \alpha_{0\eta} & \cdots & \cdots & \alpha_{k^*\eta}
\end{pmatrix},$$

$$G_\beta = \begin{pmatrix}
\beta_{11} & \cdots & \beta_{k^*1} & & & & & \\
\cdots & \cdots & \cdots & & & & & \\
\beta_{1,k_1-1} & \cdots & \beta_{k^*,k_1-1} & & & & & \\
\beta_1 & \cdots & \cdots & \cdots & \beta_k & & & \\
\beta_0 & \cdots & \cdots & \cdots & \cdots & \beta_k & & \\
 & \ddots & & & & & \ddots & \\
 & & \beta_0 & \cdots & \cdots & \cdots & \cdots & \beta_k \\
 & & & & \beta_{0,\eta-k_2+1} & \cdots & \cdots & \beta_{k^*,\eta-k_2+1} \\
 & & & & \cdots & \cdots & \cdots & \cdots \\
 & & & & \beta_{0\eta} & \cdots & \cdots & \beta_{k^*\eta}
\end{pmatrix}.$$

We suppose that G is nonsingular for each h in a suitably small right neighbourhood of zero (see [9, Chapter 4]).

Replacing U in (20) by the matrix $U^* = (U(x_1)^{\mathrm{T}},\dots,U(x_\eta)^{\mathrm{T}})^{\mathrm{T}}$ we have

$$GU^* = \Gamma + C_{p+1}h^{p+1}U^{(p+1)^*} + \mathrm{O}(h^{p+2}), \tag{22}$$

where

$$C_{p+1} = C \otimes I$$

and

$$C = \mathrm{diag}(c_{p+1}^{(1)},\dots,c_{p+1}^{(k_1-1)},\overbrace{c_{p+1},\dots,c_{p+1}}^{\eta-k+1\ \text{times}},c_{p+1}^{(\eta-k_2+1)},\dots,c_{p+1}^{(\eta)})$$

is the $\eta \times \eta$ diagonal matrix whose diagonal entries are the error constants of the local truncation errors of the η linear multistep formulas (19) and

$$U^{(p+1)^*} = (U^{(p+1)}(x_1)^{\mathrm{T}}, \ldots, U^{(p+1)}(x_\eta)^{\mathrm{T}})^{\mathrm{T}}.$$

By subtraction between (20) and (22) we obtain

$$G\Lambda = C_{p+1} h^{p+1} U^{(p+1)^*} + \mathrm{O}(h^{p+2}) \tag{23}$$

with $\Lambda = U^* - U$.

If $[x_0, x_\eta]$ is the jth shooting interval, the components of the solution Λ of linear system (23), neglecting the $\mathrm{O}(h^{p+2})$ term, are an approximation to $R_j(x_i)$, $i = (j-1)l + 1, \ldots, jl$.

In general it is not easy to compute $U^{(p+1)^*}$ on the right-hand side of (23). Only in some special cases is one able to obtain an exact form for $U^{(p+1)}(x)$ by a direct calculation or by an automatic procedure using symbolic software. For other cases, an alternative tool is furnished by the following theorem which is proved in [12].

Theorem 3.1. *Consider two different BVMs having the same order p and the same number of linear multistep formulas. Let* G, G_α, C_{p+1}, C *be the matrices defined for the former and* $\hat{G}$, $\hat{G}_\alpha$, $\hat{C}_{p+1}$, $\hat{C}$ *the corresponding matrices for the latter, while* U *and* $\hat{U}$ *are the numerical solutions obtained from the corresponding linear systems of form* (20).

If

$$\det(\hat{G}_\alpha^{-1}\hat{C} - G_\alpha^{-1}C) \neq 0,$$

then

$$h^{p+1}U^{(p+1)^*} = (\hat{G}^{-1}\hat{C}_{p+1} - G^{-1}C_{p+1})^{-1}(U - \hat{U}) + \mathrm{O}(h^{p+2})$$

for $h \in [0, h^*[$, *for some* $h^* > 0$.

4. Error estimate for the eigenvalue

According to the result established at the end of Section 1, we assume

$$\sigma_1 = s_1 = (a_2, a_1)^{\mathrm{T}} = \alpha.$$

For some initial guess μ of λ we have to solve the problem

$$\begin{aligned} &y'(x) = H(x,\mu)y(x), \\ &y(a) = \alpha. \end{aligned} \tag{24}$$

Using a BVM in conjunction with the parallel shooting, from (10) we obtain the $\mathrm{O}(h^p)$ approximations $V_{1,l}, V_{2,2l}, \ldots, V_{m,ml}$ to $V_1(\tau_1), V_2(\tau_2), \ldots, V_m(\tau_m)$. Writing $V(\mu) = V_{m,ml} \cdots V_{2,2l} V_{1,l}$, we see at once that

$$f(\mu, h) = \beta^{\mathrm{T}} V(\mu)\alpha, \tag{25}$$

where $\beta^{\mathrm{T}} = (b_1, -b_2)$. Then we approximate a solution of (12) by means of a rootfinder. If we use the Newton method we have

$$\mu_{v+1} = \mu_v - \frac{f(\mu_v, h)}{f_\mu(\mu_v, h)}, \quad v = 0, 1, \ldots, \tag{26}$$

where $f_\mu(\mu,h)=(\partial/\partial\mu)f(\mu,h)$. Thus $f_\mu(\mu,h)$ can be computed if we know $(\mathrm{d}/\mathrm{d}\mu)V(\mu)$, namely $(\mathrm{d}/\mathrm{d}\mu)V_{j,jl}$, $j=1,2,\ldots,m$.

To this end it is easy to verify from (10) that the functions $Z_j(x)=(\mathrm{d}/\mathrm{d}\mu)V_j(x)$, $j=1,2,\ldots,m$, are the solution of the IVPs

$$Z_j'(x)=H(x,\mu)Z_j(x)+Q_j(x),\quad \tau_{j-1}\leqslant x\leqslant\tau_j,$$
$$Z_j(\tau_{j-1})=0,\quad j=1,2,\ldots,m, \tag{27}$$

with $Q_j(x)$ as in (14).

With the same numerical method on the same mesh used in integrating (10) we get the $\mathrm{O}(h^p)$ approximations $Z_{j,jl}$ to $Z_j(\tau_j)$, $j=1,2,\ldots,m$.

In order to obtain an error estimate of the eigenvalue λ, we prove the following theorem.

Theorem 4.1. *Let $f(\mu,\xi)$ be analytic in μ and ξ on $|\mu-\lambda|\leqslant\epsilon$, $\xi\in[0,\xi^*[$ for some ϵ and ξ^* sufficiently small. Suppose that for any $\xi\in[0,\xi^*[$ a simple root $\mu(\xi)$ exists giving*

$$f(\mu(\xi),\xi)=0. \tag{28}$$

Then

$$\lambda-\mu(\xi)=\frac{f_\xi(\mu(\xi),\xi)}{f_\mu(\mu(\xi),\xi)}\xi+\mathrm{O}(\xi^2). \tag{29}$$

Proof. By differentiation, from (28) we have

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\mu(\xi)=-\frac{f_\xi(\mu(\xi),\xi)}{f_\mu(\mu(\xi),\xi)}. \tag{30}$$

On the other hand, recalling that $\mu(0)=\lambda$ and $f(\lambda,0)=0$,

$$f(\mu,\xi)=\sum_{v=1}^{\infty}\alpha_v(\mu)\xi^v, \tag{31}$$

where $\alpha_v(\mu)$ are also analytic in μ; thus (see, for example, [15, p. 40])

$$\mu(\xi)=\lambda+\sum_{v=1}^{\infty}\theta_v\xi^v. \tag{32}$$

The result follows from (32) and (30). □

Suppose that the numerical method used in integrating the IVPs (24) has an asymptotic error expansion given by

$$y_i=z(x_i)+\sum_{v=1}^{\infty}\gamma_{v,i}(\mu)h^{vp},$$

where y_i is the approximation to $y(x_i)$.

Then, observing that from (25) we have $f(\mu,h)=\beta^{\mathrm{T}}y_n$, Eq. (31) is obtained with $\alpha_v(\mu)=\beta^{\mathrm{T}}\gamma_{v,n}(\mu)$ and $\xi=h^p$.

Furthermore, from (29)

$$\lambda - \mu = \frac{f_\xi(\mu, \xi)}{f_\mu(\mu, \xi)} h^p + \mathrm{O}(h^{2p}). \tag{33}$$

5. Numerical experiments

Let $\lambda^{(\mathrm{s})} = \mu_v$ be an approximation to the eigenvalue λ obtained with the Newton method (26) after v iterations. We correct $\lambda^{(\mathrm{s})}$ with (33) where the $\mathrm{O}(h^{2p})$ term has been left out getting $\lambda^{(\mathrm{c})}$; namely

$$\lambda^{(\mathrm{c})} = \mu_v + \frac{f_\xi(\mu_v, \xi)}{f_\mu(\mu_v, \xi)} h^p. \tag{34}$$

Observe that in (34) the derivative $f_\mu(\mu_v, \xi)$ has been previously computed during the rootfinding process (26), while

$$f_\xi(\mu_v, \xi) \simeq \frac{f(\mu_v, \xi) - f(\mu_v, \xi/\rho^p)}{\xi - \xi/\rho^p} \tag{35}$$

for some $\rho > 1$. In (35), μ_v should be regarded as a fixed number close to the solution λ rather than as a function of h, because we are computing the partial derivative of f with respect to its second argument $\xi = h^p$ and not the total derivative of f with respect to ξ, in which we would have to take account of the dependence of μ_v on h. This conveniently means that we do not need to know $\mu_v(h/\rho)$. Thus, our approach computes f at the step size h/ρ just once, whereas computing $\mu_v(h/\rho)$ would require computing f with stepsize h/ρ many times. The extrapolation techniques used for eigenvalue improvement hitherto have generally required computation of the eiganvalue approximation at the reduced stepsize: see, for example, the SLEDGE code, [18, pp. 121, 300].

The eigenfunction corresponding to $\lambda^{(\mathrm{c})}$ is then computed following Theorem 2.1 and making use of the estimates $\tilde{e}_j(x_i)$ defined in the Remark 2.1. The discretization errors $R_j(x_i)$ are approximated by solving the linear system (23), ignoring the $\mathrm{O}(h^{p+2})$ terms.

In order to compute the solution of the problems (18) and (27), on the same shooting interval, we have selected two fourth-order BVMs: the extended trapezoidal rule (ETR) with $(2,1)$ boundary conditions ([9, p. 164])

$$\begin{aligned}
-y_0 + y_1 &= \frac{h}{24}(9f_0 + 19f_1 - 5f_2 + f_3), \\
-y_{j-1} + y_j &= \frac{h}{24}(-f_{j-2} + 13f_{j-1} + 13f_j - f_{j+1}), \quad j = 2, \ldots, \eta, \\
-y_{\eta-1} + y_\eta &= \frac{h}{24}(f_{\eta-3} - 5f_{\eta-2} + 19f_{\eta-1} + 9f_\eta),
\end{aligned} \tag{36}$$

and error constants $c_5^{(1)} = -\frac{19}{720}$, $c_5 = \frac{11}{720}$, $c_5^{(\eta)} = -\frac{19}{720}$; and the ETR_2 with $(2,1)$ boundary conditions ([9, p. 169])

$$\begin{aligned}
&\frac{1}{24}(-17y_0 + 9y_1 + 9y_2 - y_3) = \frac{h}{4}(f_0 + 3f_1),\\
&\frac{1}{12}(-y_{j-2} - 9y_{j-1} + 9y_j + y_{j+1}) = \frac{h}{2}(f_{j-1} + f_j), \quad j = 2,\ldots,\eta,\\
&\frac{1}{24}(y_{\eta-3} - 9y_{\eta-2} - 9y_{\eta-1} + 17y_\eta) = \frac{h}{4}(3f_{\eta-1} + f_\eta)
\end{aligned} \tag{37}$$

and error constants $c_5^{(1)} = -\frac{1}{80}$, $c_5 = \frac{1}{120}$, $c_5^{(\eta)} = -\frac{1}{80}$.

Even if a computer code requires, in general, the use of a variable steplength with the possibility to switch from one scheme to another, in the present context we consider a constant steplength in order to retain the analyticity of the numerical solution on μ and a theoretically simple way to apply Theorem 4.1.

The choice of the number m is dictated only by practical reasons based upon some numerical experiments. For the examples proposed we do not need to resort to a particular device for an automatic selection of m.

In the sequel, we use the following notation:

- λ_k is the kth eigenvalue of the SLP considered;
- $\lambda_k^{(\mathrm{s})}$ is the approximation μ_v to λ_k obtained from (26) with the stopping criterion given by
$$\left|\frac{f(\mu_v,h)}{f_\mu(\mu_v,h)}\right| \leqslant \varepsilon, \tag{38}$$
- $\lambda_k^{(\mathrm{c})}$ is the corrected value of $\lambda_k^{(\mathrm{s})}$;
- e_k is the n-error vector of the kth eigenfunction, i.e. the difference, on the mesh points, between the computed eigenfunction associated with $\lambda_k^{(\mathrm{c})}$ and the exact one;
- $e_k^{(\mathrm{c})}$ as above upon correction.

In the examples, for eigenvalues and eigenfunctions, we have considered as "exact" the values obtained by the SLEIGN code (see [18, Appendix C]). In (38) we have taken $\varepsilon = 10^{-7}$.

Example 1 (Paine et al. [17, p. 134]). In Table 1 we present the results for the SLP

$$-u''(x) + \mathrm{e}^x u(x) = \lambda u(x), \quad 0 \leqslant x \leqslant \pi,$$

$$u(0) = 0, \quad u(\pi) = 0.$$

The ETR_2 has been employed with the stepsize $h = \pi/400$ and $\pi/800$. We have used $m = 4$ for the eigenvalues and $m = 4$ for the eigenfunctions.

Example 2 (Paine et al. [17, p. 136]). In Table 2 we present the results for the SLP

$$-u''(x) + \frac{1}{(0.1+x)^2}u(x) = \lambda u(x), \quad 0 \leqslant x \leqslant \pi,$$

$$u(0) = 0, \quad u(\pi) = 0.$$

Table 1
Example 1

k	λ_k	$\lvert\lambda_k - \lambda_k^{(s)}\rvert$	$\lvert\lambda_k - \lambda_k^{(c)}\rvert$	$\frac{\lvert\lambda_k^{(c)} - \lambda_k^{(s)}\rvert}{\lvert\lambda_k - \lambda_k^{(s)}\rvert}$	$\frac{\lVert e_k^{(c)}\rVert}{\lVert e_k\rVert}$
1	4.8966693800	$1.18 \cdot 10^{-8}$	$1.29 \cdot 10^{-8}$	0.0880	1.0000
5	32.263707046	$1.06 \cdot 10^{-6}$	$9.09 \cdot 10^{-10}$	0.9991	1.0000
10	107.11667614	$5.98 \cdot 10^{-5}$	$1.41 \cdot 10^{-7}$	0.9976	0.2110
15	232.07881198	$6.76 \cdot 10^{-4}$	$1.57 \cdot 10^{-6}$	0.9976	0.1358
20	407.06523527	$3.79 \cdot 10^{-3}$	$8.54 \cdot 10^{-6}$	0.9977	0.0823
25	632.05890789	$1.44 \cdot 10^{-2}$	$3.12 \cdot 10^{-5}$	0.9978	0.0516
30	907.05546058	$4.33 \cdot 10^{-2}$	$8.72 \cdot 10^{-5}$	0.9979	0.0389
35	1232.0533787	$1.09 \cdot 10^{-1}$	$1.98 \cdot 10^{-4}$	0.9981	0.0456
40	1607.0520262	$2.44 \cdot 10^{-1}$	$3.78 \cdot 10^{-4}$	0.9984	0.0531
45	2032.0510984	$4.96 \cdot 10^{-1}$	$6.01 \cdot 10^{-4}$	0.9987	0.0602
50	2507.0504344	$9.37 \cdot 10^{-1}$	$7.64 \cdot 10^{-4}$	0.9991	0.0665
60	3607.0495691	$2.81 \cdot 10^{0}$	$2.68 \cdot 10^{-4}$	0.9999	0.0800
70	4907.0490473	$7.15 \cdot 10^{0}$	$6.51 \cdot 10^{-3}$	0.9990	0.1030

Table 2
Example 2

k	λ_k	$\lvert\lambda_k - \lambda_k^{(s)}\rvert$	$\lvert\lambda_k - \lambda_k^{(c)}\rvert$	$\frac{\lvert\lambda_k^{(c)} - \lambda_k^{(s)}\rvert}{\lvert\lambda_k - \lambda_k^{(s)}\rvert}$	$\frac{\lVert e_k^{(c)}\rVert}{\lVert e_k\rVert}$
1	1.5198658211	$3.29 \cdot 10^{-8}$	$1.23 \cdot 10^{-9}$	0.9624	1.0001
5	26.782863158	$4.30 \cdot 10^{-6}$	$5.56 \cdot 10^{-8}$	0.9870	0.2393
10	102.42498840	$1.25 \cdot 10^{-4}$	$4.57 \cdot 10^{-7}$	0.9963	0.0810
20	402.83423888	$7.12 \cdot 10^{-3}$	$1.40 \cdot 10^{-5}$	0.9980	0.0521
30	902.95733565	$8.02 \cdot 10^{-2}$	$1.39 \cdot 10^{-4}$	0.9982	0.0679
50	2503.0344892	$1.71 \cdot 10^{0}$	$1.71 \cdot 10^{-3}$	0.9993	0.0979
70	4903.0583616	$1.28 \cdot 10^{1}$	$9.64 \cdot 10^{-2}$	0.9925	0.1940

The ETR has been used with steps and shooting intervals as in Example 1.

Example 3 (Anderssen and de Hoog [1, p. 411]). Consider the regular SLP

$$-u''(x) + e^x u(x) = \lambda u(x), \quad 0 \leqslant x \leqslant \pi,$$

$$u(0) - u'(0) = 0, \quad u(\pi) + u'(\pi) = 0.$$

In order to estimate the discretization errors for IVPs we have applied Theorem 3.1 using the BVMs given by ETR (36) and ETR_2 (37). The step sizes used are $h = \pi/400$, $h = \pi/800$, while the number of shooting intervals is $m = 2$ for the eigenvalues and 20 for the eigenfunctions. The results obtained are given in Table 3.

Table 3
Example 3

k	λ_k	$\lvert\lambda_k - \lambda_k^{(s)}\rvert$	$\lvert\lambda_k - \lambda_k^{(c)}\rvert$	$\frac{\lvert\lambda_k^{(c)} - \lambda_k^{(s)}\rvert}{\lvert\lambda_k - \lambda_k^{(s)}\rvert}$	$\frac{\lVert e_k^{(c)}\rVert}{\lVert e_k\rVert}$
1	3.3345706250	$8.80 \cdot 10^{-9}$	$8.91 \cdot 10^{-9}$	0.0127	1.0000
5	25.567972962	$4.10 \cdot 10^{-7}$	$5.10 \cdot 10^{-10}$	0.9987	1.0000
10	89.500040998	$3.45 \cdot 10^{-5}$	$3.84 \cdot 10^{-8}$	0.9988	0.1501
20	369.35769226	$2.91 \cdot 10^{-3}$	$3.05 \cdot 10^{-6}$	0.9989	0.0606
30	849.33643726	$3.67 \cdot 10^{-2}$	$3.10 \cdot 10^{-5}$	0.9991	0.0417
50	2409.3262665	$8.58 \cdot 10^{-1}$	$1.96 \cdot 10^{-4}$	1.0002	0.0224
70	4769.3235721	$6.67 \cdot 10^{0}$	$1.40 \cdot 10^{-3}$	1.0002	0.0187

Table 4
Example 4

k	λ_k	$\lvert\lambda_k - \lambda_k^{(s)}\rvert$	$\lvert\lambda_k - \lambda_k^{(c)}\rvert$	$\frac{\lvert\lambda_k^{(c)} - \lambda_k^{(s)}\rvert}{\lvert\lambda_k - \lambda_k^{(s)}\rvert}$	$\frac{\lVert e_k^{(c)}\rVert}{\lVert e_k\rVert}$
1	0.0000000000	$1.22 \cdot 10^{-6}$	$2.05 \cdot 10^{-7}$	0.8320	1.7754
3	151.46277834	$7.10 \cdot 10^{-5}$	$1.07 \cdot 10^{-5}$	0.8486	0.9957
4	151.46322365	$3.02 \cdot 10^{-5}$	$4.43 \cdot 10^{-7}$	0.9853	2.2444
5	151.46366898	$7.52 \cdot 10^{-5}$	$9.55 \cdot 10^{-6}$	1.1270	1.0136
10	339.37066564	$6.72 \cdot 10^{-4}$	$2.63 \cdot 10^{-6}$	0.9960	2.0518
20	613.28132995	$4.85 \cdot 10^{-3}$	$1.22 \cdot 10^{-5}$	0.9974	1.0022
30	1105.7940501	$4.65 \cdot 10^{-2}$	$6.87 \cdot 10^{-5}$	0.9985	0.5007
50	2702.0797465	$9.69 \cdot 10^{-1}$	$1.00 \cdot 10^{-4}$	1.0001	0.2410
70	5101.0609909	$7.36 \cdot 10^{0}$	$1.11 \cdot 10^{-3}$	0.9998	0.1631

Example 4 (Pryce [18, p. 283, no. 7])**.** We considered the Coffey–Evans equation

$$-u''(x) + (-2\phi \cos 2x + \phi^2 \sin^2 2x)u(x) = \lambda u(x), \quad -\frac{\pi}{2} \leqslant x \leqslant \frac{\pi}{2}$$

with the boundary conditions

$$u\left(-\frac{\pi}{2}\right) = 0, \quad u\left(\frac{\pi}{2}\right) = 0.$$

We considered $\phi = 20$, $h = \pi/400$ and $\pi/800$, $m = 2$ for the eigenvalues and 20 for the eigenfunctions. As above, we used Theorem 3.1 with the ETR and ETR_2 in solving the linear system (23) for the discretization errors. The results are quoted in Table 4.

With a view to verifying the effectiveness of the technique proposed to compute the eigenvalues we consider the following examples concerning two singular SLPs where a very simple endpoint truncation procedure has been assumed.

Table 5
Example 5

k	$\lvert\lambda_k - \lambda_k^{(s)}\rvert$	$\lvert\lambda_k - \lambda_k^{(c)}\rvert$	$\frac{\lvert\lambda_k^{(c)} - \lambda_k^{(s)}\rvert}{\lvert\lambda_k - \lambda_k^{(s)}\rvert}$
1	$9.82 \cdot 10^{-7}$	$9.81 \cdot 10^{-7}$	0.0003
5	$1.47 \cdot 10^{-5}$	$1.47 \cdot 10^{-5}$	0.0030
10	$3.36 \cdot 10^{-6}$	$2.96 \cdot 10^{-6}$	0.1199
20	$3.46 \cdot 10^{-6}$	$7.79 \cdot 10^{-9}$	0.9977
30	$1.20 \cdot 10^{-5}$	$4.32 \cdot 10^{-8}$	0.9963
50	$5.66 \cdot 10^{-5}$	$2.31 \cdot 10^{-7}$	0.9959
70	$1.57 \cdot 10^{-4}$	$6.24 \cdot 10^{-7}$	0.9960

Example 5 (Pryce [18, p. 288, no. 28]). We consider the harmonic oscillator

$$-u''(x) + x^2 u(x) = \lambda u(x), \quad -\infty < x < +\infty,$$

$$u(-\infty) = 0, \quad u(+\infty) = 0,$$

whose exact eigenvalues are $\lambda_k = 2k - 1,\ k = 1, 2, \ldots$. The problem has been regularized considering the SLPs

$$-u''(x) + x^2 u(x) = \lambda u(x), \quad -b_k \leqslant x \leqslant b_k,$$

$$u(-b_k) = 0, \quad u(b_k) = 0, \quad k = 1, 2, \ldots,$$

where the endpoints depend on the eigenvalue index k following the rule

$$b_k = b\left(1 + \frac{k-1}{2m}\right), \quad k = 1, 2, \ldots$$

for some b and positive integer m. In order to keep h constant the number of shooting intervals is increasing as $m_k = m + k - 1,\ k = 1, 2, \ldots$.

In Table 5 we have quoted the results concerning the computation of the eigenvalues assuming $h = \frac{4}{750},\ b = 4,\ m = 15$ and using the ETR_2 method.

Example 6 (Pryce [18, p. 289, no. 32]). The Laguerre equation

$$-u''(x) + \left(x^2 + \frac{3}{4x^2}\right) u(x) = \lambda u(x), \quad 0 < x < +\infty,$$

$$u(0) = 0, \quad u(+\infty) = 0,$$

has the eigenvalues $\lambda_k = 4k,\ k = 1, 2, \ldots$.

We have solved the problems

$$-u''(x) + \left(x^2 + \frac{3}{4x^2}\right) u(x) = \lambda u(x), \quad 0 < a \leqslant x \leqslant b_k,$$

$$u(a) = 0, \quad u(b_k) = 0, \quad k = 1, 2, \ldots,$$

Table 6
Example 6

k	$\lvert\lambda_k - \lambda_k^{(s)}\rvert$	$\lvert\lambda_k - \lambda_k^{(c)}\rvert$	$\dfrac{\lvert\lambda_k^{(c)} - \lambda_k^{(s)}\rvert}{\lvert\lambda_k - \lambda_k^{(s)}\rvert}$
1	$7.43 \cdot 10^{-5}$	$1.02 \cdot 10^{-4}$	0.3799
5	$4.02 \cdot 10^{-3}$	$4.16 \cdot 10^{-3}$	0.0350
10	$2.84 \cdot 10^{-4}$	$5.62 \cdot 10^{-4}$	0.9810
20	$4.81 \cdot 10^{-4}$	$5.36 \cdot 10^{-5}$	1.1115
30	$6.80 \cdot 10^{-4}$	$6.49 \cdot 10^{-5}$	1.0955
50	$9.11 \cdot 10^{-4}$	$2.44 \cdot 10^{-5}$	1.0268
70	$8.09 \cdot 10^{-4}$	$1.42 \cdot 10^{-4}$	0.8237

using the ETR_2 with $h = 0.01$. We have assumed $a = 0.0001$ and

$$b_k = b\left(1 + \frac{k-1}{m}\right), \quad k = 1, 2, \ldots,$$

with $b = 4.0001$ and $m = 10$. As in the previous example we have computed λ_k using $m_k = m + k - 1$ shooting intervals in order to preserve the same value of h. The results are in Table 6.

Remark 5.1. Notice that in each of Tables 1–6, the correction technique does not seem to work as well on the lower index eigenvalues as on the higher index ones. In Examples 1–5 we believe that this is because the low-index eigenvalues are already computed to a relative accuracy which is better than square root of machine precision, and therefore difficult to improve. To confirm this, we repeated the calculations in Example 1 using the same number of shooting intervals but a much larger step size $h = \pi/100$: doing this gave $|\lambda_1 - \lambda_1^{(s)}| \simeq 1.99 \cdot 10^{-7}$ and $|\lambda_1 - \lambda_1^{(c)}| \simeq 1.04 \cdot 10^{-8}$, so in this case there is a substantial improvement even in the low-index eigenvalues. Further confirmation of the effectiveness of the technique at low indices comes from the results in Table 7 below for $k = 5$, where the correction technique is shown to yield comparable accuracy at substantially lower cost.

In Example 6 the correction technique at first appears less successful. What is actually going on here is that the interval truncation is responsible for more error than the discretization procedures.

Remark 5.2. It is worth mentioning that the value obtained for $|\lambda_k - \lambda_k^{(s)}|$ by performing the maximum iterations in (26) is, in general, greater than the value $|\lambda_k - \lambda_k^{(c)}|$ resulting from correction of the value $\lambda_k^{(s)}$ obtained with a few iterations.

To emphasize this, in Table 7 we have quoted, for Example 1, the step size and the number of iterations needed to achieve a fixed accuracy in the following cases: without correction and performing the maximum iterations in (26) and with the correction and $\varepsilon = 10^{-7}$ as stopping criterion.

Table 7
Example 1. Errors for $\lambda_k^{(s)}$ and $\lambda_k^{(c)}$; $m = 4$

k	$\lvert\lambda_k - \lambda_k^{(s)}\rvert$	$h^{(s)}$	$v^{(s)}$	$\lvert\lambda_k - \lambda_k^{(c)}\rvert$	$h^{(c)}$	$v^{(c)}$
5	$3.29 \cdot 10^{-6}$	$\frac{\pi}{300}$	6	$2.53 \cdot 10^{-6}$	$\frac{\pi}{100}$	3
	$6.92 \cdot 10^{-8}$	$\frac{\pi}{800}$	6	$7.89 \cdot 10^{-8}$	$\frac{\pi}{200}$	3
10	$1.84 \cdot 10^{-4}$	$\frac{\pi}{300}$	5	$1.29 \cdot 10^{-4}$	$\frac{\pi}{100}$	3
	$3.87 \cdot 10^{-6}$	$\frac{\pi}{800}$	4	$4.14 \cdot 10^{-6}$	$\frac{\pi}{200}$	3
15	$2.08 \cdot 10^{-3}$	$\frac{\pi}{300}$	5	$1.10 \cdot 10^{-3}$	$\frac{\pi}{100}$	2
	$4.37 \cdot 10^{-5}$	$\frac{\pi}{800}$	5	$4.71 \cdot 10^{-5}$	$\frac{\pi}{200}$	3
20	$3.79 \cdot 10^{-3}$	$\frac{\pi}{400}$	6	$2.06 \cdot 10^{-3}$	$\frac{\pi}{100}$	2
	$2.45 \cdot 10^{-4}$	$\frac{\pi}{800}$	6	$2.34 \cdot 10^{-4}$	$\frac{\pi}{200}$	2
25	$1.44 \cdot 10^{-2}$	$\frac{\pi}{400}$	5	$9.84 \cdot 10^{-3}$	$\frac{\pi}{100}$	2
	$9.36 \cdot 10^{-4}$	$\frac{\pi}{800}$	5	$7.04 \cdot 10^{-4}$	$\frac{\pi}{200}$	2
30	$1.34 \cdot 10^{-1}$	$\frac{\pi}{300}$	5	$1.35 \cdot 10^{-1}$	$\frac{\pi}{100}$	3
	$1.15 \cdot 10^{-3}$	$\frac{\pi}{1000}$	5	$1.25 \cdot 10^{-3}$	$\frac{\pi}{200}$	2

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