 CMES, vol.56, no.1, pp.85-112, 2010

The Lie-Group Shooting Method for Computing the Generalized Sturm-Liouville Problems

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Abstract: We propose a novel technique, transforming the generalized Sturm-Liouville problem: $w''+q(x,\lambda)w=0$, $a_1(\lambda)w(0)+a_2(\lambda)w'(0)=0$, $b_1(\lambda)w(1)+b_2(\lambda)w'(1)=0$ into a canonical one: $y''=f$, $y(0)=y(1)=c(\lambda)$. Then we can construct a very effective Lie-group shooting method (LGSM) to compute eigenvalues and eigenfunctions, since both the left-boundary conditions $y(0)=c(\lambda)$ and $y'(0)=A(\lambda)$ can be expressed explicitly in terms of the eigen-parameter λ. Hence, the eigenvalues and eigenfunctions can be easily calculated with better accuracy, by a finer adjusting of λ to match the right-boundary condition $y(1)=c(\lambda)$. Numerical examples are examined to show that the LGSM possesses a significantly improved performance. When comparing with exact solutions, we find that the LGSM can has accuracy up to the order of 10^{-10}.

Keywords: Generalized Sturm-Liouville problem, Eigenvalue, Eigenfunction, Lie-group shooting method, Eigen-parameter dependence boundary condition

1 Introduction

In this paper we propose a new Lie-group shooting method (LGSM) for computing the eigenvalues and eigenfunctions of the following generalized Sturm-Liouville problem:

$$\frac{d^2w(x)}{dx^2}+q(x,\lambda)w(x)=0, \quad 0<x<1, \tag{1}$$

$$a_1(\lambda)w(0)+a_2(\lambda)w'(0)=0, \tag{2}$$

$$b_1(\lambda)w(1)+b_2(\lambda)w'(1)=0. \tag{3}$$

The problem is that for the given $q(x,\lambda)$, $a_1(\lambda)$, $a_2(\lambda)$, $b_1(\lambda)$ and $b_2(\lambda)$ we need to calculate the eigenvalue λ and the eigenfunction $w(x)$. In the above we suppose

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that $q(x,\lambda) > 0$ can be arbitrarily nonlinear function of x and λ. In the latter sense, Eqs. (1)-(3) constitute a *nonlinear Sturm-Liouville problem*. When the interval is not in the range of $x \in [0,1]$ we can easily transform it into that interval by scaling the variable x.

The Sturm-Liouville problem has been of considerable physical interest and is rather important in many fields. In most cases, it is not possible to obtain all the eigenvalues of Sturm-Liouville problem analytically. For the special case of problem (1)-(3) with $q(x,\lambda) = \lambda q_1(x) + q_2(x)$ and a_1, a_2, b_1 and b_2 being constants, there are various numerical methods to approximate it. Pryce (1993) has provided a comprehensive review of the mathematical background of Sturm-Liouville problems and their numerical solutions, as well as a detailed discussion of applications. He summarized examples of Sturm-Liouville problems that have been considered by numerous authors.

There is a continuous interest in the numerical solution of Sturm-Liouville problems and associated Schrödinger equations with the aim to improve convergence rates and ease of numerical implementations of different algorithms. In order to obtain more efficient numerical results, several numerical methods have been developed in the past many years, e.g., Andrew (1994, 2000a, 2000b), Andrew and Paine (1985, 1986), Celik (2005a, 2005b), Celik and Gokmen (2005), Condon (1999), Ghelardoni (1997), Ghelardoni, Gheri and Marletta (2001, 2006), Vanden Berghe and De Meyer (1991, 1995, 2007), and Yücel (2006).

Liu (2006a, 2006b, 2006c) has expanded the group-preserving scheme (GPS) developed by Liu (2001) for ODEs to solve the nonlinear boundary value problems (BVPs), and the numerical results reveal that the Lie-group shooting method is a rather promising method to effectively solve the two-point BVPs. In the construction of the Lie-group method for the calculations of BVPs, Liu (2006a) has introduced the ideas of one-step GPS by utilizing the closure property of the Lie group and a universal mapping between two points on the cone, and hence, the new shooting method has been named the Lie-group shooting method (LGSM). At there a very important Lie-group shooting equation has been established.

Recently, Liu (2008a) could solve an inverse Sturm-Liouville problem by using a Lie group method to find the potential function $q(x)$ with high accuracy for the classical case. Moreover, the method LGSM has been modified by Liu (2008b) for the Sturm-Liouville problem, which is very effective to calculate all the eigenvalues for the classical Sturm-Liouville problems. Some applications of the LGSM can be found in Chang, Liu and Chang (2007, 2009), Liu (2008c, 2008d, 2008e, 2008f, 2008g, 2008h, 2008i), Chang, Chang and Liu (2008), Liu and Chang (2008), Liu, Chang and Chang (2008), Liu (2009), and Yeih and Liu (2009).

When the coefficient $q(x,\lambda)$ depends on the eigen-parameter λ in an arbitrarily nonlinear manner, we have a generalized Sturm-Liouville problem. This also concerns the problems with eigen-parameter dependence boundary conditions [Aliyev and Kerimov (2008); Chanane (2005, 2008); Reutskiy (2008)]. This class of problems in Eqs. (1)-(3) essentially differs from the classical one, and so far no regular method has been proposed for solving the generalized Sturm-Liouville problems. However, methods for computing the eigenvalues of the problems with eigen-parameter dependence boundary conditions have been developed by some authors [Annaby and Tharwat (2006); Aliyev and Kerimov (2008); Chanane (2005, 2007, 2008); Reutskiy (2008, 2010)]. The method presented in this paper is based on the Lie-group shooting method (LGSM), which is an extension of the previous work by Liu (2008b) to a great extent by developing a suitable LGSM to the generalized Sturm-Liouville problems.

The remaining part of this paper is arranged as follows. In Section 2 we propose a novel technique to transform the generalized Sturm-Liouville problem into a canonical form. Section 3 devotes to the construction of a one-step group preserving scheme. Based on the results in the previous two sections, we derive a Lie-group shooting equation in Section 4. Section 5 develops a closed-form solution of the unknown slope. Then the techniques of computing the eigenvalues and eigenfunctions are given in Sections 6 and 7, respectively. Numerical examples are given in Section 8. Finally, we draw some conclusions in Section 9.

2 Transformation into a canonical form

By letting

$$y(x) = [a_1 w(x) + a_2 w'(x)](1-x) + [b_1 w(x) + b_2 w'(x)]x + x(1-x) + c, \tag{4}$$

we are going to transform Eqs. (1)-(3) into a canonical form:

$$\frac{d^2 y(x)}{dx^2} = f(x, y, y'(x), \lambda), \;\; 0 < x < 1, \tag{5}$$

$$y(0) = c, \;\; y(1) = c, \tag{6}$$

where f is to be given below, and $c(\lambda) > 0$ is given in Section 6.

Taking the derivative of Eq. (4) with respect to x we have

$$y' = (b_1 - a_1)w + [b_2 - a_2 + b_1 x + a_1(1-x)]w' + [b_2 x + a_2(1-x)]w'' + 1 - 2x, \tag{7}$$

where for simplicity we omit the function variables.

Inserting Eq. (1) for w'' into the above equation, leads to

$$y' = \{b_1 - a_1 - [b_2 x + a_2(1-x)]q\}w + [b_2 - a_2 + b_1 x + a_1(1-x)]w' + 1 - 2x. \quad (8)$$

From Eqs. (4) and (8) we can solve w and w' in terms of y and y' as follows:

$$w = \frac{1}{D_1}[B_2(y - x + x^2 - c) - A_2(y' + 2x - 1)], \quad (9)$$

$$w' = \frac{1}{D_1}[A_1(y' + 2x - 1) - B_1(y - x + x^2 - c)], \quad (10)$$

where

$$A_1(x,\lambda) := a_1 + (b_1 - a_1)x,$$
$$A_2(x,\lambda) := a_2 + (b_2 - a_2)x,$$
$$B_1(x,\lambda) := b_1 - a_1 - qA_2,$$
$$B_2(x,\lambda) := b_2 - a_2 + A_1,$$
$$D_1(x,\lambda) := A_1B_2 - A_2B_1 = A_1^2 + qA_2^2 + a_1b_2 - a_2b_1. \quad (11)$$

The term D_1 can be guaranteed to be positive. If $a_1b_2 - a_2b_1 < 0$, we can multiply Eq. (2) or Eq. (3) by -1, which does not change the boundary conditions, such that $-[a_1b_2 - a_2b_1] > 0$, and hence, $D_1 > 0$.
Further taking the derivative of Eq. (10) with respect to x we have

$$\begin{aligned} w'' =& \frac{1}{D_1}[A_1(y'' + 2) + (b_1 - a_1)(y' + 2x - 1) - B_3(y - x + x^2 - c) - B_1(y' + 2x - 1)] \\ &- \frac{D_2}{D_1^2}[A_1(y' + 2x - 1) - B_1(y - x + x^2 - c)], \end{aligned} \quad (12)$$

where

$$D_2(x,\lambda) := \frac{\partial D_1}{\partial x} = 2A_1(b_1 - a_1) + 2qA_2(b_2 - a_2) + q_x A_2^2,$$
$$B_3(x,\lambda) := \frac{\partial B_1}{\partial x} = -q_x A_2 - (b_2 - a_2)q, \quad (13)$$

with q_x denoting $\partial q(x,\lambda)/\partial x$.
From Eqs. (1), (9) and (12) it follows that

$$y'' = \frac{D_2}{D_1}(y' + 2x - 1) - \frac{1}{A_1}\left[\frac{B_1D_2}{D_1} + qB_2 - B_3\right](y - x + x^2 - c) - 2, \quad (14)$$

which is just our desired form in Eq. (5).

We can transform Eqs. (14) and (6) into an equivalent first-order ODEs' system:

$$
\begin{aligned}
&u_1' = u_2,\\
&u_2' = f(x,u_1,u_2,\lambda),\\
&u_1(0) = c, \;\; u_1(1) = c,
\end{aligned}
\tag{15}
$$

where $u_1 = y$ and $u_2 = y'$, and

$$
f(x,u_1,u_2,\lambda) := \frac{D_2}{D_1}(u_2+2x-1) - \frac{1}{A_1}\left[\frac{B_1 D_2}{D_1} + qB_2 - B_3\right](u_1 - x + x^2 - c) - 2.
\tag{16}
$$

The advantage by adjusting the original very complex boundary conditions equal to $u_1(0) = u_1(1) = c > 0$ will be demonstrated in Section 4, and the advantage by adding an extra term $x(1-x)$ in Eq. (4) will be explained in Section 5.

If $a_1 = 0$, then $A_1 = 0$ when $x = 0$. For this case we need to use

$$
f(x=0,u_1,u_2,\lambda) := \frac{D_2}{D_1}(u_2-1) + \frac{1}{b_1}\left[\frac{B_1 D_2}{D_1} + qB_2 - B_3\right] - 2
\tag{17}
$$

for the initial value of f.

The present approach of generalized Sturm-Liouville problem is based on the group preserving scheme (GPS) developed by Liu (2001) for the integration of initial value problems (IVPs). The GPS method is very effective to deal with ordinary differential equations (ODEs) endowing with special structures as shown by Liu (2005) for stiff equations, and by Liu (2006d) for ODEs with constraints.

The stepping techniques developed for IVPs require both the initial conditions of u_1 and u_2 for two first-order ODEs. If the initial value of u_2 is available, then we can numerically integrate the following IVP step-by-step in a forward direction from $x = 0$ to $x = 1$:

$$
u_1' = u_2, \tag{18}
$$

$$
u_2' = f(x,u_1,u_2,\lambda), \tag{19}
$$

$$
u_1(0) = c, \tag{20}
$$

$$
u_2(0) = A. \tag{21}
$$

The shooting technique is simply finding a suitable A, such that the solution of $u_1(x)$ can also match the right-boundary condition $u_1(1) = c$. In Section 6 we can derive explicit forms of A and c in terms of the eigen-parameter λ.

3 One-step GPS

3.1 The GPS

Let us write Eqs. (18) and (19) in a vector form:

$$\mathbf{u}' = \mathbf{f}(x, \mathbf{u}, \lambda), \tag{22}$$

where

$$\mathbf{u} := \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}, \ \mathbf{f} := \begin{bmatrix} u_2 \\ f(x, u_1, u_2, \lambda) \end{bmatrix}. \tag{23}$$

Liu (2001) has embedded Eq. (22) into an augmented system:

$$\mathbf{X}' := \frac{d}{dx} \begin{bmatrix} \mathbf{u} \\ \|\mathbf{u}\| \end{bmatrix} = \begin{bmatrix} \mathbf{0}_{2\times 2} & \frac{\mathbf{f}(x,\mathbf{u},\lambda)}{\|\mathbf{u}\|} \\ \frac{\mathbf{f}^{\mathrm{T}}(x,\mathbf{u},\lambda)}{\|\mathbf{u}\|} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \|\mathbf{u}\| \end{bmatrix} := \mathbf{A}\mathbf{X}, \tag{24}$$

where $\mathbf{A}$ is an element of the Lie algebra $so(2,1)$ satisfying

$$\mathbf{A}^{\mathrm{T}}\mathbf{g} + \mathbf{g}\mathbf{A} = \mathbf{0} \tag{25}$$

with

$$\mathbf{g} = \begin{bmatrix} \mathbf{I}_2 & \mathbf{0}_{2\times 1} \\ \mathbf{0}_{1\times 2} & -1 \end{bmatrix} \tag{26}$$

a Minkowski metric. Here, $\mathbf{I}_2$ is an identity matrix, and the superscript T stands for the transpose.

The augmented vector $\mathbf{X}$ satisfies the cone condition:

$$\mathbf{X}^{\mathrm{T}}\mathbf{g}\mathbf{X} = \mathbf{u}\cdot\mathbf{u} - \|\mathbf{u}\|^2 = 0. \tag{27}$$

To preserve it, Liu (2001) has developed a group-preserving scheme (GPS):

$$\mathbf{X}_{k+1} = \mathbf{G}(k)\mathbf{X}_k, \tag{28}$$

where $\mathbf{X}_k$ denotes the numerical value of $\mathbf{X}$ at the discrete x_k, and $\mathbf{G}(k) \in SO_o(2,1)$ satisfies

$$\mathbf{G}^{\mathrm{T}}\mathbf{g}\mathbf{G} = \mathbf{g}, \tag{29}$$

$$\det \mathbf{G} = 1, \tag{30}$$

$$G_0^0 > 0, \tag{31}$$

where G_0^0 is the 00th component of $\mathbf{G}$.

The main contribution of Liu (2001) is given a general ODE three sructures: a geometric structure of cone, a Lie-algebra structure, and a Lie-group structure. There are many Lie-group integrators which can be developed for Eq. (24) to preserve the above three structures; see, for example, Liu (2007), and Lee and Liu (2009).

3.2 Generalized mid-point rule

Applying scheme (28) to Eq. (24) with a specified initial condition $\mathbf{X}(0) = \mathbf{X}_0$ we can compute the solution $\mathbf{X}(x)$ by GPS. Assuming that the stepsize used in GPS is $\Delta x = 1/K$, and starting from an initial augmented condition $\mathbf{X}_0 = \mathbf{X}(0) = (\mathbf{u}_0^{\mathrm{T}}, \|\mathbf{u}_0\|)^{\mathrm{T}}$ we can calculate the value $\mathbf{X}(1) = (\mathbf{u}^{\mathrm{T}}(1), \|\mathbf{u}(1)\|)^{\mathrm{T}}$ at $x = 1$ by

$$\mathbf{X}_f = \mathbf{G}_K(\Delta x) \cdots \mathbf{G}_1(\Delta x)\mathbf{X}_0. \tag{32}$$

However, let us recall that each $\mathbf{G}_i$, $i = 1, \ldots, K$, is an element of the Lie group $SO_o(2,1)$, and by the closure property of the Lie group, $\mathbf{G}_K(\Delta x) \cdots \mathbf{G}_1(\Delta x)$ is also a Lie group denoted by $\mathbf{G}$. Hence, we have

$$\mathbf{X}_f = \mathbf{G}\mathbf{X}_0. \tag{33}$$

This is a one-step Lie-group transformation from $\mathbf{X}_0$ to $\mathbf{X}_f$.

Usually it is very hard to obtain an exact solution of $\mathbf{G}$. To be an approximation, we can calculate $\mathbf{G}$ by a generalized mid-point rule, which is obtained from an exponential mapping of $\mathbf{A}$ by taking the values of the argument variables of $\mathbf{A}$ at a generalized mid-point. The Lie group generated from this constant $\mathbf{A} \in so(2,1)$ admits a closed-form representation:

$$\mathbf{G} = \begin{bmatrix} \mathbf{I}_2 + \frac{(a-1)}{\|\hat{\mathbf{f}}\|^2}\hat{\mathbf{f}}\hat{\mathbf{f}}^{\mathrm{T}} & \frac{b\hat{\mathbf{f}}}{\|\hat{\mathbf{f}}\|} \\ \frac{b\hat{\mathbf{f}}^{\mathrm{T}}}{\|\hat{\mathbf{f}}\|} & a \end{bmatrix}, \tag{34}$$

where

$$\hat{\mathbf{u}} = r\mathbf{u}_0 + (1-r)\mathbf{u}_f, \tag{35}$$

$$\hat{\mathbf{f}} = \mathbf{f}(\hat{x}, \hat{\mathbf{u}}, \lambda), \tag{36}$$

$$a = \cosh\left(\frac{\|\hat{\mathbf{f}}\|}{\|\hat{\mathbf{u}}\|}\right), \tag{37}$$

$$b = \sinh\left(\frac{\|\hat{\mathbf{f}}\|}{\|\hat{\mathbf{u}}\|}\right). \tag{38}$$

Here, we use the initial $\mathbf{u}_0$ and the final $\mathbf{u}_f$ through a suitable weighting factor r to calculate $\mathbf{G}$, where $0 < r < 1$ is a parameter and $\hat{x} = r$. The above method employed a generalized mid-point rule to calculate $\mathbf{G}$, and the resultant is a single-parameter Lie group element $\mathbf{G}(r)$.

3.3 A Lie group mapping between two points on the cone

Let us define a new vector

$$\mathbf{F} := \frac{\hat{\mathbf{f}}}{\|\hat{\mathbf{u}}\|}, \tag{39}$$

such that Eqs. (34), (37) and (38) can also be expressed as

$$\mathbf{G} = \begin{bmatrix} \mathbf{I}_2 + \frac{a-1}{\|\mathbf{F}\|^2}\mathbf{F}\mathbf{F}^{\mathrm{T}} & \frac{b\mathbf{F}}{\|\mathbf{F}\|} \\ \frac{b\mathbf{F}^{\mathrm{T}}}{\|\mathbf{F}\|} & a \end{bmatrix}, \tag{40}$$

$$a = \cosh(\|\mathbf{F}\|), \tag{41}$$

$$b = \sinh(\|\mathbf{F}\|). \tag{42}$$

From Eqs. (33) and (40) it follows that

$$\mathbf{u}_f = \mathbf{u}_0 + \eta \mathbf{F}, \tag{43}$$

$$\|\mathbf{u}_f\| = a\|\mathbf{u}_0\| + b\frac{\mathbf{F}\cdot\mathbf{u}_0}{\|\mathbf{F}\|}, \tag{44}$$

where

$$\eta := \frac{(a-1)\mathbf{F}\cdot\mathbf{u}_0 + b\|\mathbf{u}_0\|\|\mathbf{F}\|}{\|\mathbf{F}\|^2}. \tag{45}$$

Substituting

$$\mathbf{F} = \frac{1}{\eta}(\mathbf{u}_f - \mathbf{u}_0) \tag{46}$$

into Eq. (44) we obtain

$$\frac{\|\mathbf{u}_f\|}{\|\mathbf{u}_0\|} = a + b\frac{(\mathbf{u}_f - \mathbf{u}_0)\cdot\mathbf{u}_0}{\|\mathbf{u}_f - \mathbf{u}_0\|\|\mathbf{u}_0\|}, \tag{47}$$

where

$$a = \cosh\left(\frac{\|\mathbf{u}_f - \mathbf{u}_0\|}{\eta}\right), \tag{48}$$

$$b = \sinh\left(\frac{\|\mathbf{u}_f - \mathbf{u}_0\|}{\eta}\right) \tag{49}$$

are obtained by inserting Eq. (46) for $\mathbf{F}$ into Eqs. (41) and (42).

Let

$$\cos\theta := \frac{[\mathbf{u}_f - \mathbf{u}_0] \cdot \mathbf{u}_0}{\|\mathbf{u}_f - \mathbf{u}_0\| \|\mathbf{u}_0\|}, \tag{50}$$

$$S := \|\mathbf{u}_f - \mathbf{u}_0\|, \tag{51}$$

and from Eqs. (47)-(49) it follows that

$$\frac{\|\mathbf{u}_f\|}{\|\mathbf{u}_0\|} = \cosh\left(\frac{S}{\eta}\right) + \cos\theta \sinh\left(\frac{S}{\eta}\right). \tag{52}$$

By defining

$$Z := \exp\left(\frac{S}{\eta}\right), \tag{53}$$

from Eq. (52) we can obtain a quadratic equation for Z:

$$(1+\cos\theta)Z^2 - \frac{2\|\mathbf{u}_f\|}{\|\mathbf{u}_0\|}Z + 1 - \cos\theta = 0. \tag{54}$$

The solution is found to be

$$Z = \frac{\frac{\|\mathbf{u}_f\|}{\|\mathbf{u}_0\|} + \sqrt{\left(\frac{\|\mathbf{u}_f\|}{\|\mathbf{u}_0\|}\right)^2 - 1 + \cos^2\theta}}{1+\cos\theta}, \tag{55}$$

and then from Eqs. (53) and (51) we obtain

$$\eta = \frac{\|\mathbf{u}_f - \mathbf{u}_0\|}{\ln Z}. \tag{56}$$

Therefore, between any two points $(\mathbf{u}_0, \|\mathbf{u}_0\|)$ and $(\mathbf{u}_f, \|\mathbf{u}_f\|)$ on the cone, there exists a Lie group element $\mathbf{G} \in SO_o(2,1)$ mapping $(\mathbf{u}_0, \|\mathbf{u}_0\|)$ onto $(\mathbf{u}_f, \|\mathbf{u}_f\|)$, which is given by

$$\begin{bmatrix} \mathbf{u}_f \\ \|\mathbf{u}_f\| \end{bmatrix} = \mathbf{G} \begin{bmatrix} \mathbf{u}_0 \\ \|\mathbf{u}_0\| \end{bmatrix}, \tag{57}$$

where $\mathbf{G}$ is uniquely determined by $\mathbf{u}_0$ and $\mathbf{u}_f$ through Eqs. (40)-(42), (46) and (56).

4 The Lie-group shooting method

The generalized Sturm-Liouville problem considered in Section 1 requires both the information at the initial point $x = 0$ and at the terminal point $x = 1$. However, the usual stepping scheme requires a complete information at the starting point $x = 0$. Some effort is then required to reconcile the stepping scheme for the integration of Sturm-Liouville problem presented by Eqs. (5) and (6).

From Eqs. (18)-(21) it follows that

$$u_1' = u_2, \tag{58}$$

$$u_2' = f(x, u_1, u_2, \lambda), \tag{59}$$

$$u_1(0) = c, \;\; u_1(1) = c, \tag{60}$$

$$u_2(0) = A, \;\; u_2(1) = B, \tag{61}$$

where A and B are two supplemented unknowns, and $c > 0$ is given below.

From Eqs. (46), (60) and (61) it follows that

$$\mathbf{F} := \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} = \frac{1}{\eta} \begin{bmatrix} 0 \\ B-A \end{bmatrix}. \tag{62}$$

By inserting Eq. (23) for $\mathbf{u}$ into Eqs. (56), (55) and (50) we can obtain

$$\eta = \frac{\sqrt{(A-B)^2}}{\ln Z}, \tag{63}$$

$$Z = \frac{\frac{\sqrt{c^2+B^2}}{\sqrt{c^2+A^2}} + \sqrt{\frac{c^2+B^2}{c^2+A^2} - 1 + \cos^2\theta}}{1+\cos\theta}, \tag{64}$$

$$\cos\theta = \frac{A(B-A)}{\sqrt{(A-B)^2}\sqrt{c^2+A^2}}. \tag{65}$$

When compare Eq. (62) with Eq. (39), and with the aid of Eqs. (35), (36) and (58)-(61) we obtain

$$rA + (1-r)B = 0, \tag{66}$$

$$A - B + \frac{\eta}{\xi}\hat{f} = 0, \tag{67}$$

where

$$\hat{f} := f(r, c, rA + (1-r)B, \lambda) = f(r, c, 0, \lambda), \tag{68}$$

$$\xi := \sqrt{c^2 + [rA + (1-r)B]^2} = c, \tag{69}$$

because of $\hat{u}_1 = c$ and $\hat{u}_2 = rA + (1-r)B = 0$.

Eq. (66) is a crucial result for the further development of a closed-form formula about A. This equation is obtained by using the two identical boundary values of $u_1 = y$ in Eq. (15). From the above equations we can see that the advantage by adjusting the two boundary values in Eq. (15) to be equal is that we can derive Eq. (66), and that a closed-form solution of A will be available in the next section.

5 The solution of A

From Eqs. (66)-(68), (16), and (69) we can obtain an algebraic equation for A:

$$Ac + \eta_0 f_1 = 0, \tag{70}$$

where

$$f_1(r) = f(r, c, 0, \lambda), \tag{71}$$

$$Z = \frac{\sqrt{c^2 + B^2} + \sqrt{B^2}}{\sqrt{c^2 + A^2} - \sqrt{A^2}}, \tag{72}$$

$$\eta_0 = \frac{\sqrt{A^2}}{\ln Z}. \tag{73}$$

Here, $B = rA/(r-1)$ has a different sign from A because of $0 < r < 1$.

Eq. (70) can be used to solve A for a given r. If A is available, we can return to integrate Eqs. (18)-(21) by a suitable forward IVP solver.

Without adding an extra term $x(1-x)$ in Eq. (4), the three terms $2x-1$, x^2-x and -2 will disappear from Eq. (16), which in turns make $\hat{f} = 0$ by viewing Eqs. (16) and (68), because of $\hat{u}_1 = c$ and $\hat{u}_2 = 0$. Under this condition we only have $A = 0$ by Eq. (70), because of $f_1 = 0$ and $c > 0$. Therefore, we have added an extra term $x(1-x)$ in Eq. (4) to avoid $\hat{f} = 0$.

More interestingly, Eq. (70) can be solved analytically for A. Here we consider only the case of $A > 0$. For this case inserting Eq. (73) for η_0 into Eq. (70) we can obtain

$$\ln Z = \frac{-f_1}{c}. \tag{74}$$

Upon defining

$$f_2(r) := \exp\left(-\frac{f_1(r)}{c}\right), \tag{75}$$

and substituting Eq. (72) for Z into Eq. (74) we obtain

$$\frac{\sqrt{c^2+B^2}+\sqrt{B^2}}{\sqrt{c^2+A^2}-\sqrt{A^2}}=f_2. \tag{76}$$

Eq. (76) can be written as

$$f_2A-B=f_2\sqrt{c^2+A^2}-\sqrt{c^2+B^2} \tag{77}$$

by using $A>0$ and $B<0$. Squaring the above equation and cancelling the common terms we can rearrange it to

$$2f_2\sqrt{c^2+B^2}\sqrt{c^2+A^2}=(1+f_2^2)c^2+2f_2AB. \tag{78}$$

Squaring again and cancelling the common term and factor we can get

$$4f_2^2(A^2+B^2)-4f_2(1+f_2^2)AB=(1-f_2^2)^2c^2. \tag{79}$$

Inserting $B=rA/(r-1)$ and through some algebraic manipulations we eventually obtain:

$$\frac{4f_2}{(r-1)^2}[f_2-(1-f_2)^2r^2+(1-f_2)^2r]A^2=(1-f_2^2)^2c^2. \tag{80}$$

If the following condition holds

$$f_3(r):=f_2-(1-f_2)^2r^2+(1-f_2)^2r>0, \tag{81}$$

then A has a positive solution:

$$A=\sqrt{\frac{(r-1)^2(1-f_2^2)^2c^2}{4f_2f_3}}. \tag{82}$$

6 Computing eigenvalues

In the previous section we have derived a closed-form solution to calculate the slope A for each r in its admissible range. If A is available, then we can apply the fourth-order Runge-Kutta method (RK4) to integrate Eqs. (18)-(21). Up to this point we should note that the Lie-group shooting method is an exact technique without making any assumption of the approximation in the derivations of all required formulae.

In principle, if there exists one solution w of Eqs. (1) and (2), there are many solutions of the type αw, $\alpha\in\mathbb{R}$. Assume that one of these solutions has a slope $w'(0)\neq 0$ at the left-end, then there are many different solutions with slopes $\alpha w'(0)$, $\alpha\in\mathbb{R}$.

It means that the slope A can be an arbitrary value. So the factor r in Eq. (82) can be any value in the interval of $r \in (0,1)$. Hence, we can fix $r = 1/2$, and then we come to the following equation for A:

$$A = \sqrt{\frac{(1-f_4^2)^2 c^2}{4(1+f_4^2)^2 f_4}}, \tag{83}$$

where

$$f_4(\lambda) := \exp\left(\frac{2}{c} - \frac{1}{4cA_1(1/2,\lambda)}\left[\frac{B_1(1/2,\lambda)D_2(1/2,\lambda)}{D_1(1/2,\lambda)} + q(1/2,\lambda)B_2(1/2,\lambda) - B_3(1/2,\lambda)\right]\right). \tag{84}$$

Here A is only dependent on λ. In order to avoid f_4 to be a tiny value in the calculation of large eigenvalues, we can take

$$c = \left|2 - \frac{1}{4A_1(1/2,\lambda)}\left[\frac{B_1(1/2,\lambda)D_2(1/2,\lambda)}{D_1(1/2,\lambda)} + q(1/2,\lambda)B_2(1/2,\lambda) - B_3(1/2,\lambda)\right]\right|, \tag{85}$$

such that $f_4 = \exp(\pm 1)$ dependent on the sign of the argument.

In order to calculate the eigenvalues we can let λ run in a selected interval we are interesting, and then insert λ into Eqs. (83) and (85) we can obtain A and c. When c and A are given, we can calculate $y(1)$ by integrating Eqs. (18)-(21). Therefore, we can plot a curve of the variation of $y(1) - c$ with respect to λ, namely the eigenvalues curve, of which the intersecting points with the zero line give the values of the required eigenvalues. In order to obtain more accurate eigenvalue we can adjust the λ nearby the marked one until $y(1)$ satisfies $|y(1) - c| < \varepsilon_1$, where ε_1 is a given tolerance of error of mismatching the right-boundary condition $y(1) = c$.

7 Calculating eigenfunctions and identification of accuracy

When the eigenvalue λ is calculated in the previous section by the LGSM, we can insert it into Eq. (85) to calculate c, and then into Eq. (83) to calculate A. After that we are easily calculate u_1 and u_2 in the whole interval by a suitable numerical integration method, say, the RK4, to integrate Eqs. (18)-(21).

If u_1 and u_2 are available we can calculate the eigenfunction $w(x)$ and its first two derivatives by

$$w = \frac{1}{D_1}[B_2(u_1 - x + x^2 - c) - A_2(u_2 + 2x - 1)], \tag{86}$$

$$w' = \frac{1}{D_1}[A_1(u_2 + 2x - 1) - B_1(u_1 - x + x^2 - c)], \tag{87}$$

$$w'' = \frac{1}{D_1}[A_1\{f(x,u_1,u_2,\lambda) + x\} + (b_1 - a_1)(u_2 + 2x - 1) - B_3(u_1 - x + x^2 - c) \\ - B_1(u_2 + 2x - 1)] - \frac{D_2}{D_1^2}[A_1(u_2 + 2x - 1) - B_1(u_1 - x + x^2 - c)]. \tag{88}$$

In order to check the accuracy of the obtained eigenvalue and eigenfunction, we use the following three criteria to investigate the performance of the LGSM:

$$\text{Equation Error} := |w''(x) + qw(x)|, \tag{89}$$

$$\text{Left Boundary Error} := |a_1 w(0) + a_2 w'(0)|, \tag{90}$$

$$\text{Right Boundary Error} := |b_1 w(1) + b_2 w'(1)|. \tag{91}$$

Below we will use the LGSM to find eigenvalues and corresponding eigenfunctions for some examples appeared in the literature.

8 Numerical examples

8.1 Example 1

For a first and simple test example inspired by Aliyev and Kerimov (2008) we consider the eigen-parameter dependence boundary condition of a Sturm-Liouville eigenvalues problem with $a_1 = 0$, $a_2 = 1$, $b_1 = \lambda - \lambda^2/\pi^2$, $b_2 = 1$ and $q = \lambda$:

$$-w''(x) = \lambda w(x), \;\; 0 < x < 1, \tag{92}$$

$$w'(0) = 0, \;\; \left(\lambda - \frac{\lambda^2}{\pi^2}\right) w(1) + w'(1) = 0. \tag{93}$$

We apply the Lie-group shooting method (LGSM) in Section 6 to calculate the eigenvalues in a range of $0 < \lambda < 25$. From Fig. 1(a) it can be seen that the curve of $y(1) - c$ is intersected with the zero line at five points. In this calculation the stepsize used in the RK4 is $\Delta x = 0.001$. We will fix this stepsize for all later calculations by using the RK4.

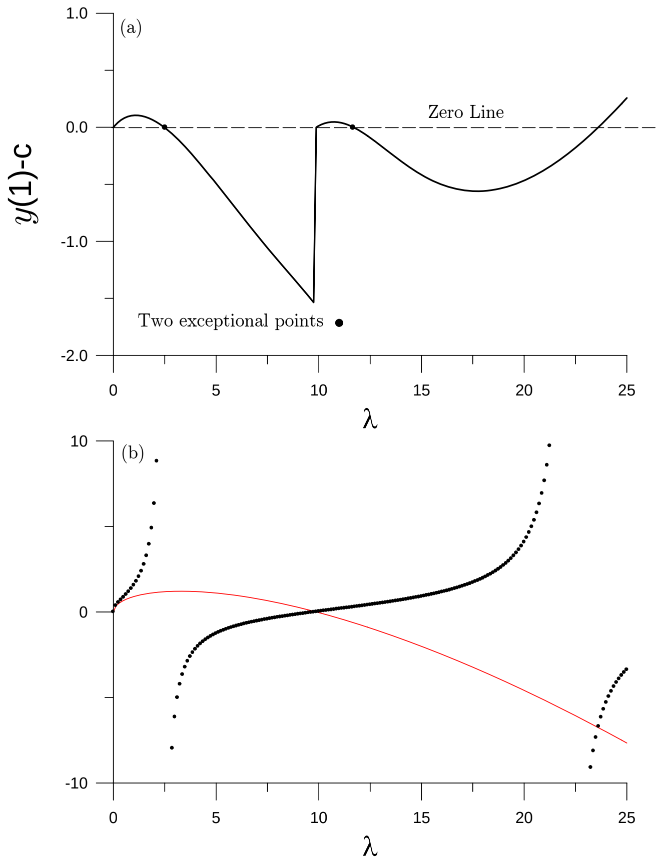

Figure 1: For Example 1: (a) plotting the eigenvalues curve, and (b) the two curves determine the eigenvalues.

As demonstrated by Aliyev and Kerimov (2008), $\lambda = 0$ is a double eigenvalue, $\lambda = \pi^2$ is a simple eigenvalue and all other simple eigenvalues are the roots of the following equation:

$$\tan\sqrt{\lambda} = \sqrt{\lambda}\left(1 - \frac{\lambda^2}{\pi^2}\right). \tag{94}$$

Therefore, for comparison purpose we also plot the curves of the above two functions in Fig. 1(b) by the dotted points, whose intersecting points are the roots. The results are coincident with the zero points in Fig. 1(a). However, it is very interesting that the second and the fourth zero points as marked by black solid points in Fig. 1(a) are not the intersecting points in Fig. 1(b). These two points are exceptional from Eq. (94).

In order check our algorithm for the generation of the second exceptional point, we use the following two criteria to investigate the accuracy of the LGSM:

$$\text{Equation Error} := |w''(x) + \lambda w(x)|, \tag{95}$$

$$\text{Right Boundary Error} := \left| \left(\lambda - \frac{\lambda^2}{\pi^2} \right) w(1) + w'(1) \right|. \tag{96}$$

When we found the eigenvalue $\lambda = 11.6924379$ by the LGSM, the corresponding eigenfunction $w(x)$ can be calculated by Eq. (86), and the first two derivatives by Eqs. (87) and (88).

We find that the Right Boundary Error is very small in the order of 4.7×10^{-9}, and the Equation Error is plotted in Fig. 2. Very accurately, the error is in the order of 10^{-17}.

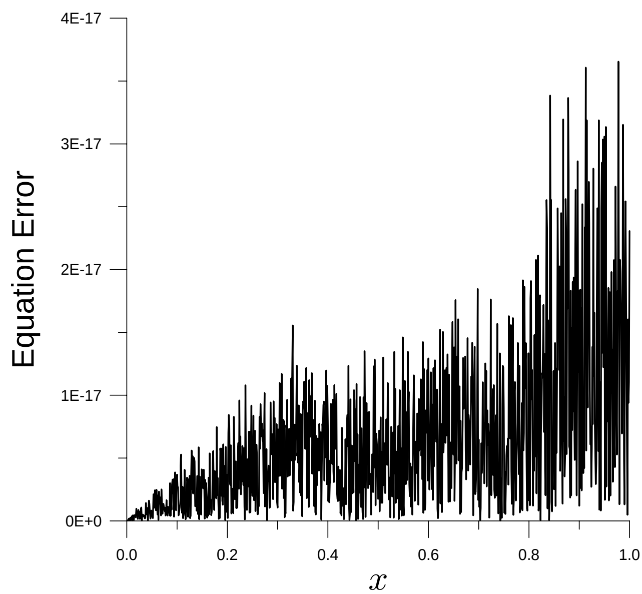

Figure 2: Showing the Equation Error for the fourth eigenvalue of Example 1.

8.2 Example 2

The following test example is taken from Binding and Browne (1997), and Chanane (2005):

$$w''(x) + \lambda w(x) = 0, \ \ 0 < x < 1, \tag{97}$$

$$w(0) + (\lambda - 4\pi^2)w'(0) = 0, \ \ w(1) - \lambda w'(1) = 0. \tag{98}$$

Here we have $a_1 = 1$, $a_2 = \lambda - 4\pi^2$, $b_1 = 1$, $b_2 = -\lambda$, and $q = \lambda$.
When we apply the LGSM to calculate the eigenvalues in a range of $0 < \lambda < 160$, we can see that the curve of $[y(1) - c]/|y(1) - c|$ is intersected with the zero line at many points as shown in Fig. 3. But, in Table 3.1 of the paper by Chanane (2005), only three eigenvalues are reported.

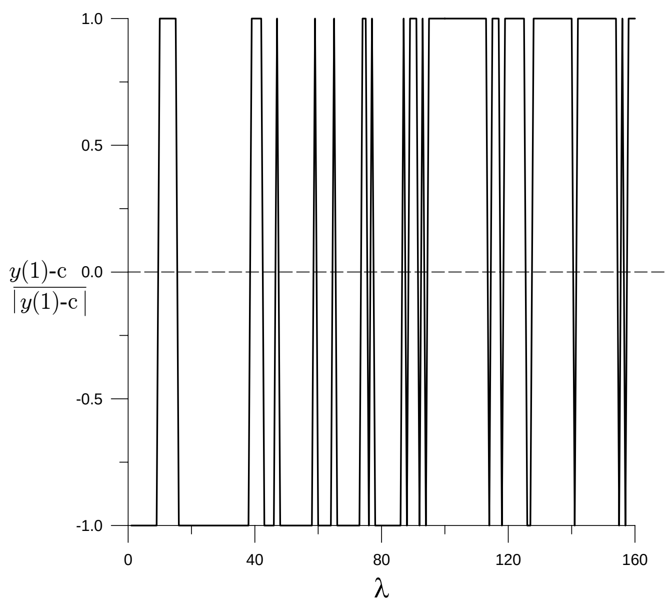

Figure 3: Displaying the eigenvalue curve for Example 2.

When we found the first eigenvalue $\lambda = 9.7308865$ by the LGSM, the corresponding eigenfunction $w(x)$ can be calculated by Eq. (86), and the first two derivatives by Eqs. (87) and (88). We find that the Left Boundary Error is very small in the order of 2.17×10^{-19}, and the Right Boundary Error is in the order of 6.3×10^{-10}. The Equation Error is plotted in Fig. 4(a), which is very accurate with the error in the order of 10^{-18}. We also plotted the corresponding eigenfunction $w(x)$ in

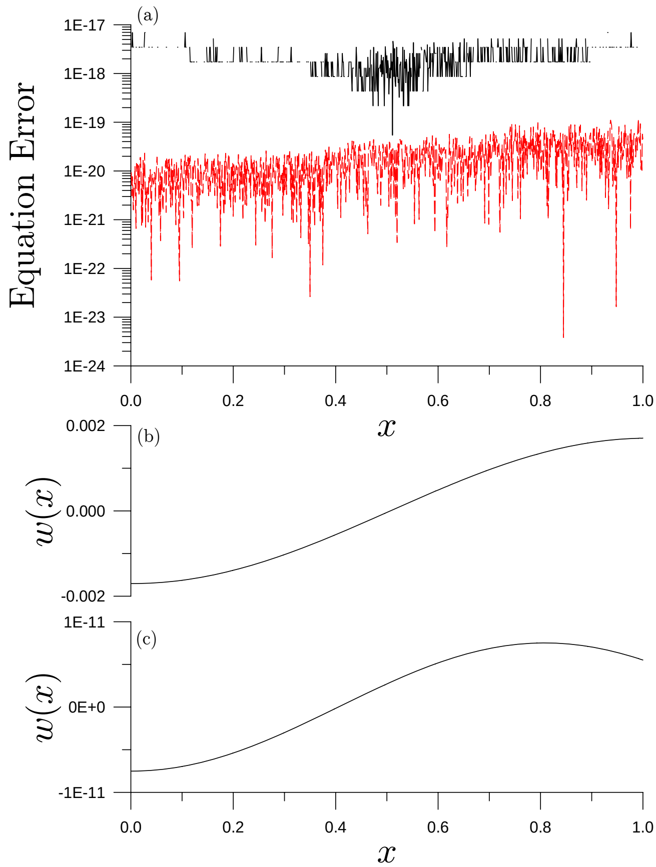

Figure 4: For Example 2: (a) plotting the Equation Errors, and the eigenfunctions corresponding to (b) the first eigenvalue, and (c) the second eigenvalue.

Fig. 4(b). The second eigenvalue is $\lambda = 15.20906425$. The Equation Error is plotted in Fig. 4(a) by the dashed line, which is very accurate with the error in the order of 10^{-20}, and the corresponding eigenfunction $w(x)$ is also plotted in Fig. 4(c).

In order to pick up the eigenvalues more precisely, we can plot the eigenvalue curve of $[y(1)-c]/|y(1)-c|$ in a finer range, as shown in Fig. 5(a) in the range of $[38,45]$. It can be seen that the distribution of eigenvalues is very complex. When we found one eigenvalue $\lambda = 44.70035341243$ by the LGSM, the Left Boundary Error is zero, and the Right Boundary Error is in the order of 3.3×10^{-10}. The Equation Error is plotted in Fig. 5(b), which is very accurate with the error in the order of 10^{-12}. The corresponding eigenfunction $w(x)$ is plotted in Fig. 5(c), which is very different from the one plotted in Fig. 4(b).

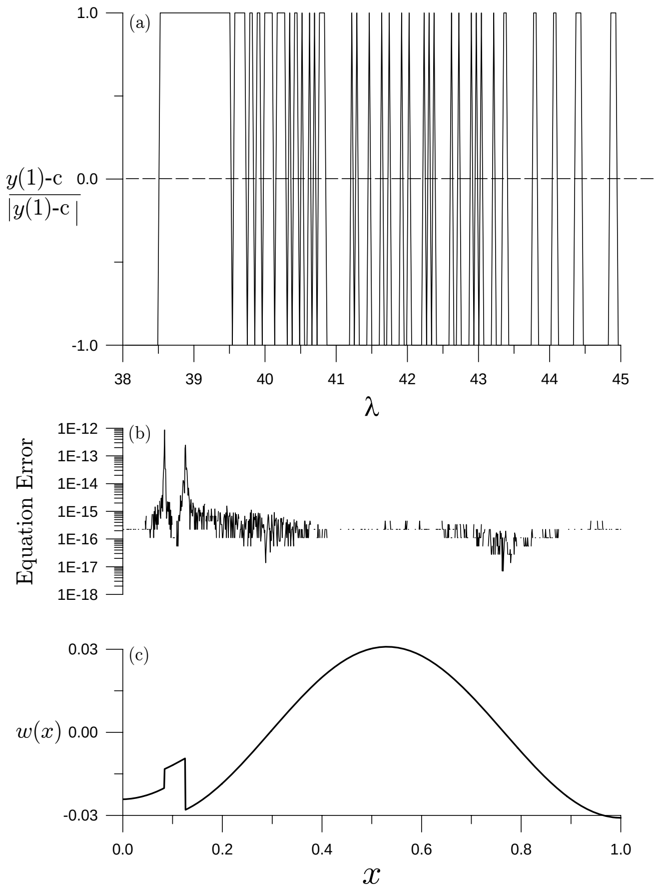

Figure 5: For Example 2: (a) displaying the eigenvalue curve, (b) plotting the Equation Error, and (c) the eigenfunction for a certain eigenvalue.

Remark: Chanane (2005) by using the sampling method only found three eigenvalues in the range of $[0,160]$, and indeed, the first eigenvalue he gave in the above paper is not accurate than the present one when comparing with the exact eigenvalue. The LGSM shows that for this example the distribution of eigenvalues is very complex. With a refined tunning of the parameter λ to match the right boundary condition $y(1) = c(\lambda)$, we can find very accurate results.

8.3 Example 3

The following example is taken from Chanane (2005) and Reutskiy (2008):

$$w''(x) + (\lambda - e^x)w(x) = 0, \;\; 0 < x < 1, \tag{99}$$

$$w(0) = 0, \;\; -\sqrt{\lambda}\sin\sqrt{\lambda}w(1) + \cos\sqrt{\lambda}w'(1) = 0. \tag{100}$$

So we have $a_1 = 1$, $a_2 = 0$, $b_1 = -\sqrt{\lambda}\sin\sqrt{\lambda}$, $b_2 = \cos\sqrt{\lambda}$, and $q = \lambda - e^x$.

When we apply the LGSM to calculate the eigenvalues in a range of $0 < \lambda < 80$, we can see that the curve of $[y(1)-c]/|y(1)-c|$ is intersected with the zero line at many points as shown in Fig. 6(a). But, in Table 3.4 of the paper by Chanane (2005), and in Table 5 of the paper by Reutskiy (2008) only six eigenvalues are reported.

For the eigenvalue $\lambda = 0.519996736312803$ obtained by the LGSM, the Right Boundary Error has error in the order of 1.4×10^{-12}, and the Equation Error is plotted in Fig. 6(b), which is very accurate with the error in the order of 10^{-13}. The corresponding eigenfunction $w(x)$ is plotted in Fig. 6(c). This eigenfunction has a sharp variation near the right-end, and is almost zero in the range of $[0, 0.948]$.

The above two papers are all given the first eigenvalue near to 0.92906. However, we find that it is the second eigenvalue with $\lambda_2 = 0.92906202858$. We identify that the Right Boundary Error is in the order of 1.2×10^{-12}, and the Equation Error as plotted in Fig. 6(b) by the dashed line is in the order of 10^{-16}. The corresponding eigenfunction $w(x)$ is plotted in Fig. 6(c) by the dashed line, which is very different from the the first one. As compared with the result obtained by Chanane (2005), the accuracy in the finding of eigenvalue is raised from 6.75×10^{-9} to 10^{-12}.

8.4 Example 4

The following example is taken from Reutskiy (2008, 2010):

$$w''(x) + \frac{w(x)}{(\lambda + x^2)^2} = 0, \;\; 0 < x < 1, \tag{101}$$

$$w(0) = w(1) = 0. \tag{102}$$

Here $q = 1/(\lambda + x^2)^2$ is a nonlinear function of the eigen-parameter λ.

When we apply the LGSM to calculate the eigenvalues in a range of $0 < \lambda < 0.2$, we can see that the curve of $[y(1)-c]/|y(1)-c|$ is intersected with the zero line at ten points as shown in Fig. 7(a), of which the number of eigenvalues is coincident with that obtained by Reutskiy (2008, 2010).

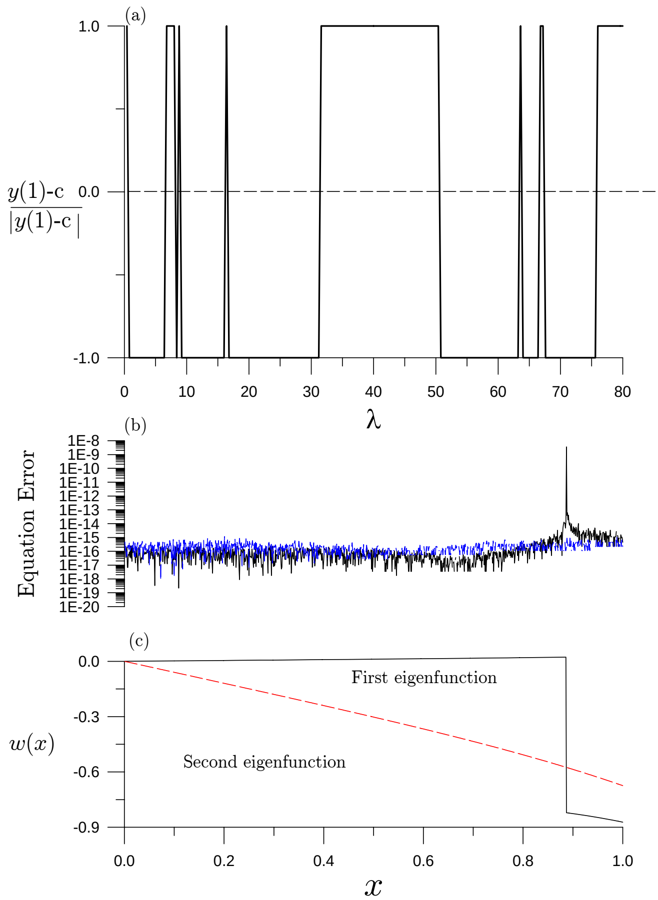

Figure 6: For Example 3: (a) displaying the eigenvalue curve, (b) plotting the Equation Errors, and (c) the eigenfunctions for two certain eigenvalues.

For the first eigenvalue $\lambda = 0.0010636506102$ and the fifth eigenvalue $\lambda = 0.006301140338$ we plot the corresponding eigenfunctions in Figs. 7(b) and 7(c), respectively. The eigenvalues we calculate have the accuracy over 10^{-10}, which are better than that calculated by Reutskiy (2008, 2010). The eigenfunctions $w(x)$ as plotted in Fig. 7 have different scales and oscillatory behaviors for different modes.

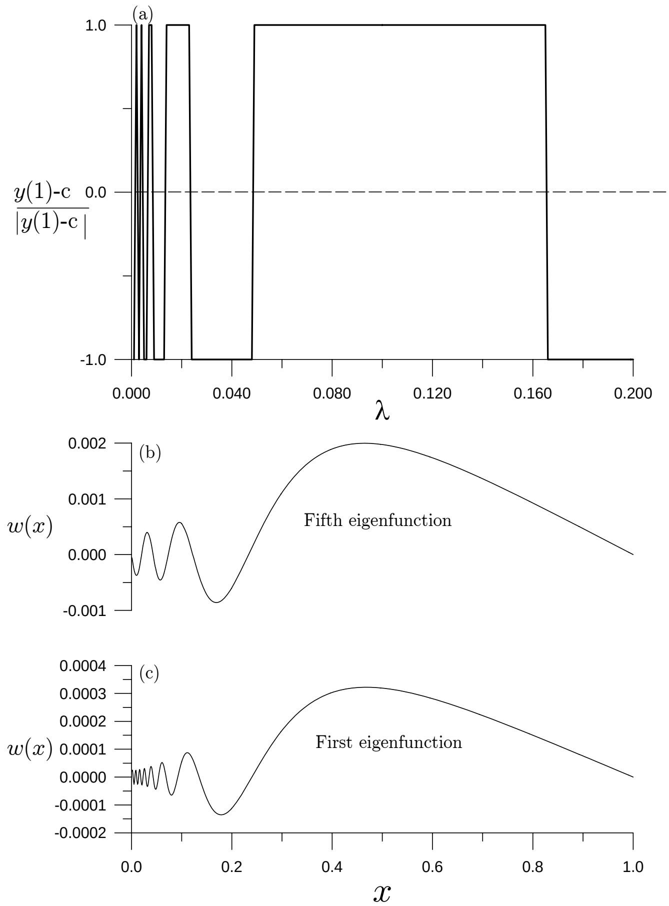

Figure 7: For Example 4: (a) displaying the eigenvalue curve, (b) plotting the fifth eigenfunction, and (c) plotting the first eigenfunction.

8.5 Example 5

The following example is taken from Reutskiy (2010):

$$w''(x)+\frac{w(x)}{(\lambda+x)^2}=0,\ \ 0<x<1, \tag{103}$$

$$w(0)=w(1)=0. \tag{104}$$

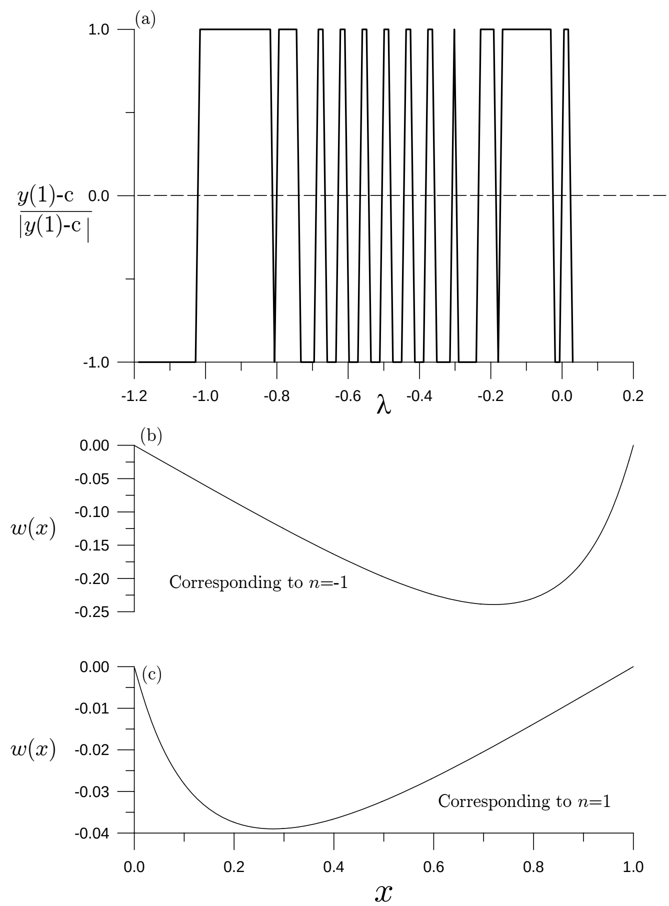

Figure 8: For Example 5: (a) displaying the eigenvalue curve, (b) plotting the eigenfunction corresponding to $n = -1$, and (c) plotting the eigenfunction corresponding to $n = 1$.

This problem has closed-form solutions:

$$w = \text{const} \times \left(1 + \frac{x}{\lambda}\right)^{1/2} \sin\left[\frac{\pi}{\gamma} \ln\left(1 + \frac{x}{\lambda}\right)\right], \tag{105}$$

$$\lambda_n = \frac{1}{\exp(\gamma n) - 1}, \quad \gamma = \frac{2\pi}{\sqrt{3}}. \tag{106}$$

Table 1 shows the results for $n = -1$ and $n = 1$, which are compared with the results obtained by Reutskiy (2010).

When we apply the LGSM to calculate the eigenvalues in a range of $-1.2 < \lambda <$

Table 1: Comparing the eigenvalues for Example 5 with those of Reutskiy (2010)

n	Reutskiy	Present	Exact
-1	-1.0272981	-1.027305717791	-1.027305717634675
1	0.02729809	0.02730571779926	0.027305717634675

0.03, we can see that the curve of $[y(1)-c]/|y(1)-c|$ is intersected with the zero line at many points as shown in Fig. 8(a).

For the eigenvalues $\lambda = -1.027305717791$ and $\lambda = 0.02730571779926$ we plot the corresponding eigenfunctions in Figs. 8(b) and 8(c), respectively. The eigenvalues we calculate have the accuracy in the order of 10^{-10}, which are better than those calculated by Reutskiy (2010).

9 Conclusions

The key point to succeed the Lie-group shooting method (LGSM) for the generalized Sturm-Liouville problem is the variable transformation given in Eq. (4), which is a novel transformation, including both w and w' on the right-hand side. The LGSM developed here can easily calculate the eigenvalues and eigenfunctions of generalized Sturm-Liouville problems, which is due to the relations $y(0) = c(\lambda)$ and $y'(0) = A(\lambda)$ given in Eqs. (85) and (83). Five numerical examples with eigenparameter dependence boundary conditions and nonlinear potential functions were given to confirm the efficiency and accuracy of the present Lie-group shooting approach, which is much easy to implement with low computational cost than the numerical methods appeared in other literature. Moreover, the accuracy assessed by the Equation Error and Boundary Errors are improved significiantly. Because our method is very effective, many eigenvalues, which were not found previously by other methods, could be delicately detected by the LGSM in the present paper.

Acknowledgement: Taiwan's National Science Council Project NSC-97-2221-E-002-264-MY3 granted to the author is highly appreciated.

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