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A Lie-Group Shooting Method for Computing Eigenvalues and Eigenfunctions of Sturm-Liouville Problems

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Abstract: For the Sturm-Liouville eigenvalues problem we construct a very effective Lie-group shooting method (LGSM) to search the eigenvalues, and when eigenvalue is determined we can also search a missing left-boundary condition of the slope through a weighting factor $r \in (0,1)$. Hence, the eigenvalues and eigenfunctions can be calculated with a better accuracy. Because a closed-form formula is derived to calculate unknown slope in terms of λ for the estimation of eigenvalues, the present method is easy to implement and has a low computational cost. Similarly by applying the LGSM to find a corresponding eigenfunction in terms of λ is easily carried out in a finer range of r. Numerical examples were examined to show that the Lie-group shooting method has a significantly improved accuracy than before.

Keyword: Sturm-Liouville eigenvalues problem, Eigenvalue, Eigenfunction, Lie-group shooting method

1 Introduction

The Sturm-Liouville eigenvalues problem has been of considerable physical interest and is rather important in many fields, including partial differential equations, vibration of continuum mechanics, and quantum mechanics.

In most cases, it is not possible to obtain the eigenvalues of Sturm-Liouville eigenvalues problem analytically. However, there are various numerical methods to approximate it. Pryce (1993) has provided an excellent review of the mathematical background of Sturm-Liouville eigenvalues problems and their numerical solutions, as well as a detailed discussion of applications. He summarized examples of Sturm-Liouville eigenvalues problems that have been considered by numerous authors.

There is a continued interest in the numerical solution of Sturm-Liouville eigenvalues problems and associated Schrödinger equations with the aim to improve convergence rates and ease of implementation of different algorithms. In order to obtain more efficient numerical results, several numerical methods have been developed in the past several years, e.g., Andrew (1994, 2000a), 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). Among, the most influential one is the algebraically asymptotic correction method, which is reviewed by Andrew (2000).

Although Ghelardoni and Gheri (2001) have discussed a shooting technique for computing eigenvalues, to our best knowledge there is no study on the Lie-group shooting method to Sturm-Liouville eigenvalues problem. In this paper we propose a new shooting method for computing the eigenvalues and eigenfunctions of the following Sturm-Liouville eigenvalues problem:

$$-\frac{d}{dx}\left[p(x)\frac{dy(x)}{dx}\right]+q(x)y(x)=\lambda s(x)y(x), \quad x_0<x<x_f, \tag{1}$$

$$y(x_0)=0, \quad y(x_f)=0. \tag{2}$$

The problem is that for the given $p(x)$, $q(x)$ and $s(x)$ we need to calculate the eigenvalue λ and eigenfunction $y(x)$. In the above we suppose $p(x)$, $q(x)$, $s(x)$ continuous with $p(x)$ and $s(x)$ strictly

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positive. When x_0 and x_f are finite the Sturm-Liouville eigenvalues problem is regular; otherwise, it is singular.

By letting

$$x = x_0 + (x_f - x_0)t, \tag{3}$$

$$u(t) = y(x) + t(1-t) + c, \tag{4}$$

where c is a given positive constant, we can transform Eqs. (1) and (2) into an equivalent system:

$$\begin{aligned}\ddot{u}(t) = &-\frac{\dot{p}(t)}{p(t)}[\dot{u}(t)+2t-1] \\ &+\frac{(x_f-x_0)^2}{p(t)}[q(t)-\lambda s(t)][u(t)-t(1-t)-c] \\ &-2,\end{aligned} \tag{5}$$

$$u(0) = c, \quad u(1) = c. \tag{6}$$

The advantage by adjusting the original zero boundary values equal to $c > 0$ will be demonstrated in Section 3, and the advantage by adding an extra term $t(1-t)$ in Eq. (4) will be explained in Section 4. Here, $p(t)$, $q(t)$ and $s(t)$ should be understood as $p(x(t))$, $q(x(t))$ and $s(x(t))$.

The present approach of Sturm-Liouville eigenvalues 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 (2006a) for ODEs with constraints.

The stepping techniques developed for IVPs require both the initial conditions of $u_1 = u$ and $u_2 = \dot{u}$ for the second-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 $t = 0$ to $t = 1$:

$$\dot{u}_1 = u_2, \tag{7}$$

$$\dot{u}_2 = f(t, u_1, u_2), \tag{8}$$

$$u_1(0) = c, \tag{9}$$

$$u_2(0) = A, \tag{10}$$

where

$$\begin{aligned}f(t,u_1,u_2) := &-\frac{\dot{p}(t)}{p(t)}[u_2(t)+2t-1] \\ &+\frac{(x_f-x_0)^2}{p(t)}[q(t)-\lambda s(t)][u_1(t)-t(1-t)-c] \\ &-2.\end{aligned} \tag{11}$$

Here, we call Eqs. (7)-(10) the $(\mathbf{u},t)$-IVP, where $\mathbf{u}(t) = (u_1(t), u_2(t))$ denotes the system variables in the t-domain. The shooting technique is simply by finding a suitable A, such that the solution of $u_1(t)$ can also match the right-boundary condition $u_1(1) = c$.

Liu (2006b, 2006c, 2006d) has extended the GPS for ODEs to solve the 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. Recently, Liu (2008) could solve an inverse Sturm-Liouville problem by using a Lie group method to find the potential function $q(x)$ with high accuracy. In the construction of Lie-group method for the calculations of BVPs, Liu (2006b) has introduced the idea of one-step GPS by utilizing the closure property of Lie group, and hence, the new shooting method has been named the Lie-group shooting method. However, this method needs to be modified for the Sturm-Liouville problem.

2 One-step GPS

2.1 The GPS

Let us write Eqs. (7) and (8) in a vector form:

$$\dot{\mathbf{u}} = \mathbf{f}(t, \mathbf{u}), \tag{12}$$

where

$$\mathbf{u} := \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}, \quad \mathbf{f} := \begin{bmatrix} u_2 \\ f(t,u_1,u_2) \end{bmatrix}. \tag{13}$$

Liu (2001) has embedded Eq. (12) into an augmented system:

$$\dot{\mathbf{X}} := \frac{d}{dt}\begin{bmatrix}\mathbf{u}\\ \|\mathbf{u}\|\end{bmatrix} = \begin{bmatrix}\mathbf{0}_{2\times 2} & \frac{\mathbf{f}(t,\mathbf{u})}{\|\mathbf{u}\|}\\ \frac{\mathbf{f}^{\mathrm{T}}(t,\mathbf{u})}{\|\mathbf{u}\|} & 0\end{bmatrix}\begin{bmatrix}\mathbf{u}\\ \|\mathbf{u}\|\end{bmatrix} := \mathbf{A}\mathbf{X}, \tag{14}$$

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

$$\mathbf{A}^{\mathrm{T}}\mathbf{g} + \mathbf{g}\mathbf{A} = \mathbf{0} \tag{15}$$

with

$$\mathbf{g} = \begin{bmatrix}\mathbf{I}_2 & \mathbf{0}_{2\times 1}\\ \mathbf{0}_{1\times 2} & -1\end{bmatrix} \tag{16}$$

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

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

$$\mathbf{X}^{\mathrm{T}}\mathbf{g}\mathbf{X} = \mathbf{u}\cdot\mathbf{u} - \|\mathbf{u}\|^2 = 0. \tag{17}$$

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

$$\mathbf{X}_{k+1} = \mathbf{G}(k)\mathbf{X}_k, \tag{18}$$

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

$$\mathbf{G}^{\mathrm{T}}\mathbf{g}\mathbf{G} = \mathbf{g}, \tag{19}$$

$$\det \mathbf{G} = 1, \tag{20}$$

$$G_0^0 > 0, \tag{21}$$

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

The main contribution of Liu (2001) is given a general ODE three structures: 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. (14) to preserve the above three structures; see, for example, Liu (2007).

2.2 Generalized mid-point rule

Applying scheme (18) to Eq. (14) with a specified initial condition $\mathbf{X}(0) = \mathbf{X}_0$ we can compute the solution $\mathbf{X}(t)$ by GPS. Assuming that the stepsize used in GPS is $\Delta t = 1/K$, 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 $t = 1$ by

$$\mathbf{X}_f = \mathbf{G}_K(\Delta t)\cdots\mathbf{G}_1(\Delta t)\mathbf{X}_0. \tag{22}$$

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 Lie group, $\mathbf{G}_K(\Delta t)\cdots\mathbf{G}_1(\Delta t)$ is also a Lie group denoted by $\mathbf{G}$. Hence, we have

$$\mathbf{X}_f = \mathbf{G}\mathbf{X}_0. \tag{23}$$

This is a one-step 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 $\mathbf{A} \in so(2,1)$ is known to be an element of the proper orthochronous Lorentz group, which admits a closed-form representation:

$$\mathbf{G} = \begin{bmatrix}\mathbf{I}_2 + \frac{(a-1)}{\|\hat{\mathbf{f}}\|^2}\hat{\mathbf{f}}\hat{\mathbf{f}}^{\mathrm{T}} & \frac{b\hat{\mathbf{f}}}{\|\hat{\mathbf{f}}\|}\\ \frac{b\hat{\mathbf{f}}^{\mathrm{T}}}{\|\hat{\mathbf{f}}\|} & a\end{bmatrix}, \tag{24}$$

where

$$\hat{\mathbf{u}} = r\mathbf{u}_0 + (1-r)\mathbf{u}_f, \tag{25}$$

$$\hat{\mathbf{f}} = \mathbf{f}(\hat{t}, \hat{\mathbf{u}}), \tag{26}$$

$$a = \cosh\left(\frac{\|\hat{\mathbf{f}}\|}{\|\hat{\mathbf{u}}\|}\right), \tag{27}$$

$$b = \sinh\left(\frac{\|\hat{\mathbf{f}}\|}{\|\hat{\mathbf{u}}\|}\right). \tag{28}$$

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 $\hat{t} = r$. The above method employed a generalized mid-point rule to calculate $\mathbf{G}$, and the resultant is a single-parameter Lie group element $\mathbf{G}(r)$.

2.3 A Lie group mapping between two points on the cone

Let us define a new vector

$$\mathbf{F} := \frac{\hat{\mathbf{f}}}{\|\hat{\mathbf{u}}\|}, \tag{29}$$

such that Eqs. (24), (27) and (28) can also be expressed as

$$\mathbf{G} = \begin{bmatrix} \mathbf{I}_2 + \frac{a-1}{\|\mathbf{F}\|^2}\mathbf{F}\mathbf{F}^{\mathrm{T}} & \frac{b\mathbf{F}}{\|\mathbf{F}\|} \\ \frac{b\mathbf{F}^{\mathrm{T}}}{\|\mathbf{F}\|} & a \end{bmatrix}, \tag{30}$$

$$a = \cosh(\|\mathbf{F}\|), \tag{31}$$

$$b = \sinh(\|\mathbf{F}\|). \tag{32}$$

From Eqs. (23) and (30) it follows that

$$\mathbf{u}_f = \mathbf{u}_0 + \eta\mathbf{F}, \tag{33}$$

$$\|\mathbf{u}_f\| = a\|\mathbf{u}_0\| + b\frac{\mathbf{F}\cdot\mathbf{u}_0}{\|\mathbf{F}\|}, \tag{34}$$

where

$$\eta := \frac{(a-1)\mathbf{F}\cdot\mathbf{u}_0 + b\|\mathbf{u}_0\|\|\mathbf{F}\|}{\|\mathbf{F}\|^2}. \tag{35}$$

Substituting

$$\mathbf{F} = \frac{1}{\eta}(\mathbf{u}_f - \mathbf{u}_0) \tag{36}$$

into Eq. (34) we obtain

$$\frac{\|\mathbf{u}_f\|}{\|\mathbf{u}_0\|} = a + b\frac{(\mathbf{u}_f - \mathbf{u}_0)\cdot\mathbf{u}_0}{\|\mathbf{u}_f - \mathbf{u}_0\|\|\mathbf{u}_0\|}, \tag{37}$$

where

$$a = \cosh\left(\frac{\|\mathbf{u}_f - \mathbf{u}_0\|}{\eta}\right), \tag{38}$$

$$b = \sinh\left(\frac{\|\mathbf{u}_f - \mathbf{u}_0\|}{\eta}\right) \tag{39}$$

are obtained by inserting Eq. (36) for $\mathbf{F}$ into Eqs. (31) and (32).

Let

$$\cos\theta := \frac{[\mathbf{u}_f - \mathbf{u}_0]\cdot\mathbf{u}_0}{\|\mathbf{u}_f - \mathbf{u}_0\|\|\mathbf{u}_0\|}, \tag{40}$$

$$S := \|\mathbf{u}_f - \mathbf{u}_0\|, \tag{41}$$

and from Eqs. (37)-(39) it follows that

$$\frac{\|\mathbf{u}_f\|}{\|\mathbf{u}_0\|} = \cosh\left(\frac{S}{\eta}\right) + \cos\theta\sinh\left(\frac{S}{\eta}\right). \tag{42}$$

By defining

$$Z := \exp\left(\frac{S}{\eta}\right), \tag{43}$$

we obtain a quadratic equation for Z from Eq. (42):

$$(1+\cos\theta)Z^2 - \frac{2\|\mathbf{u}_f\|}{\|\mathbf{u}_0\|}Z + 1 - \cos\theta = 0. \tag{44}$$

The solution is found to be

$$Z = \frac{\frac{\|\mathbf{u}_f\|}{\|\mathbf{u}_0\|} + \sqrt{\left(\frac{\|\mathbf{u}_f\|}{\|\mathbf{u}_0\|}\right)^2 - 1 + \cos^2\theta}}{1+\cos\theta}, \tag{45}$$

and then from Eqs. (43) and (41) we obtain

$$\eta = \frac{\|\mathbf{u}_f - \mathbf{u}_0\|}{\ln Z}. \tag{46}$$

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

$$\begin{bmatrix} \mathbf{u}_f \\ \|\mathbf{u}_f\| \end{bmatrix} = \mathbf{G}\begin{bmatrix} \mathbf{u}_0 \\ \|\mathbf{u}_0\| \end{bmatrix}, \tag{47}$$

where $\mathbf{G}$ is uniquely determined by $\mathbf{u}_0$ and $\mathbf{u}_f$ through Eqs. (30)-(32), (36) and (46).

3 The Lie-group shooting method

The Sturm-Liouville eigenvalues problem considered in Section 1 requires both the information at the initial point $t = 0$ and at the terminal point $t = 1$. However, the usual time stepping scheme requires a complete information at the starting point $t = 0$. Some effort is then required to reconcile the stepping scheme for the integration of Sturm-Liouville eigenvalues problem presented there.

From Eqs. (7)-(10) it follows that

$$\dot{u}_1 = u_2, \tag{48}$$

$$\dot{u}_2 = f(t, u_1, u_2), \tag{49}$$

$$u_1(0) = c, \quad u_1(1) = c, \tag{50}$$

$$u_2(0) = A, \quad u_2(1) = B, \tag{51}$$

where A and B are two supplemented unknown constants, and c is a given positive constant.

From Eqs. (36), (50) and (51) it follows that

$$\mathbf{F} := \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} = \frac{1}{\eta} \begin{bmatrix} 0 \\ B-A \end{bmatrix}. \tag{52}$$

By inserting Eq. (13) for $\mathbf{u}$ into Eqs. (46), (45) and (40) we can obtain

$$\eta = \frac{\sqrt{(A-B)^2}}{\ln Z}, \tag{53}$$

$$Z = \frac{\frac{\sqrt{c^2+B^2}}{\sqrt{c^2+A^2}} + \sqrt{\frac{c^2+B^2}{c^2+A^2} - 1 + \cos^2\theta}}{1+\cos\theta}, \tag{54}$$

$$\cos\theta = \frac{A(B-A)}{\sqrt{(A-B)^2}\sqrt{c^2+A^2}}. \tag{55}$$

When compare Eq. (52) with Eq. (29), and with the aid of Eqs. (25), (26) and (48)-(51) we obtain

$$rA + (1-r)B = 0, \tag{56}$$

$$A - B + \frac{\eta}{\xi}\hat{f} = 0, \tag{57}$$

where

$$\hat{f} := f(r, c, rA + (1-r)B) = f(r, c, 0), \tag{58}$$

$$\xi := \sqrt{c^2 + [rA + (1-r)B]^2} = c, \tag{59}$$

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

Eq. (56) 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 $u_1 = u$ in Eq. (6). From the above equations we can see that c must be a positive value, and the advantage by adjusting the two boundary values in Eq. (6) equal is that we can derive Eq. (56), and that a closed-form solution of A will be available as follows.

The above derivation of the governing equations (53)-(59) is based on by equating the two $\mathbf{F}$'s in Eqs. (29) and (36). It also means that the two Lie groups defined by Eqs. (24) and (30) are equal. Under this sense we may call our shooting technique a Lie-group shooting method (LGSM).

4 The solution of A

From Eqs. (56)-(58), (11), and (59) we obtain an algebraic equation for A:

$$Ac + \eta_0 f_1 = 0, \tag{60}$$

where

$$f_1(r) = -\frac{\dot{p}(r)}{p(r)}(2r-1) - \frac{(x_f - x_0)^2 r(1-r)}{p(r)}[q(r) - \lambda s(r)] - 2, \tag{61}$$

$$Z = \frac{\sqrt{c^2+B^2} + \sqrt{B^2}}{\sqrt{c^2+A^2} - \sqrt{A^2}}, \tag{62}$$

$$\eta_0 = \frac{\sqrt{A^2}}{\ln Z}. \tag{63}$$

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

Eq. (60) can be used to solve A for a given r. If A is available, we can return to integrate Eqs. (7)-(10) by a suitable forward IVP solver.

Without adding an extra term $t(1-t)$ in Eq. (4), the two terms $-t(1-t)$ and -2 will disappear from Eq. (11), which in turns make $\hat{f} = 0$ by viewing Eqs. (11) and (58) for the case of $\dot{p} = 0$ because of $\hat{u}_1 = c$. Under this condition we only have $A = 0$ by Eq. (57). Therefore, we have added an extra term $t(1-t)$ in Eq. (4) to avoid $\hat{f} = 0$.

More interestingly, Eq. (60) can be solved analytically for A. Here we consider only the case of $A > 0$. For this case inserting Eq. (63) for η_0 into Eq. (60) we obtain

$$\ln Z = \frac{-f_1}{c}. \tag{64}$$

Defining

$$f_2(r) := \exp\left(-\frac{f_1(r)}{c}\right), \tag{65}$$

and substituting Eq. (62) for Z into Eq. (64) we obtain

$$\frac{\sqrt{c^2+B^2} + \sqrt{B^2}}{\sqrt{c^2+A^2} - \sqrt{A^2}} = f_2. \tag{66}$$

Eq. (66) can be written as

$$f_2A - B = f_2\sqrt{c^2+A^2} - \sqrt{c^2+B^2} \tag{67}$$

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

$$2f_2\sqrt{c^2+B^2}\sqrt{c^2+A^2} = (1+f_2^2)c^2 + 2f_2AB. \tag{68}$$

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

$$4f_2^2(A^2+B^2) - 4f_2(1+f_2^2)AB = (1-f_2^2)^2c^2. \tag{69}$$

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

$$\frac{4f_2}{(r-1)^2}[f_2 - (1-f_2)^2r^2 + (1-f_2)^2r]A^2 = (1-f_2^2)^2c^2. \tag{70}$$

If the following condition holds

$$f_3(r) := f_2 - (1-f_2)^2r^2 + (1-f_2)^2r > 0, \tag{71}$$

then A has a positive solution:

$$A = \sqrt{\frac{(r-1)^2(1-f_2^2)^2c^2}{4f_2f_3}}. \tag{72}$$

5 Calculating 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 the $(\mathbf{u},t)$-IVP in Eqs. (7)-(10). 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 y of Eqs. (1) and (2), there are many solutions of the type αy, $\alpha \in \mathbb{R}$. Assume that one of these solutions has a slope $y'(x_0) \neq 0$ (it should be nonzero; otherwise we have only a trivial solution $y = 0$) at the left-end, then there are many different solutions with slopes $\alpha y'(x_0)$, $\alpha \in \mathbb{R}$. It means that the slope A can be an arbitrary value. So the factor r in Eq. (72) can be any value in the interval of $r \in (0,1)$. Now, we can fix $r = 1/2$, and then we come to the following equation for A:

$$A = \sqrt{\frac{(1-f_4^2)^2c^2}{4(1+f_4^2)^2f_4}}, \tag{73}$$

where

$$f_4(\lambda) := \exp\left(\frac{(x_f-x_0)^2}{4cp(1/2)}[q(1/2)-\lambda s(1/2)] + \frac{2}{c}\right). \tag{74}$$

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

$$c = \left|\frac{(x_f-x_0)^2}{4p(1/2)}[q(1/2)-\lambda s(1/2)]+2\right|, \tag{75}$$

such that $f_4 = \exp(\pm 1)$ dependent on the sign of the argument $(x_f - x_0)^2[q(1/2) - \lambda s(1/2)]/[4p(1/2]+2$.

In order to calculate the eigenvalues we let λ run in a selected interval we are interesting, and then insert λ into Eqs. (73) and (75) we can obtain A and c. When c and A are given, we can calculate $y(x_f)$ by integrating Eqs. (7)-(10) and using Eq. (4). Therefore, we can plot a curve of the variation of $y(x_f)$ 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 $y(x_f)$ satisfies $|y(x_f)| < \varepsilon_1$, where ε_1 is a given tolerance of error of mismatching the right-boundary condition $y(x_f) = 0$.

6 Calculating eigenfunctions

When the eigenvalue λ is calculated in the previous section, we can insert it into Eq. (72) to calculate A. However, how to determine a correct r requires a numerical integration of the ODEs.

For a trial r in the admissible range, we can calculate A and then numerically integrate Eqs. (7)-(10) from $t = 0$ to $t = 1$, obtaining $y(x_f)$ by Eq. (4), and compare the end value of $y^r(x_f)$ with the exact one $y(x_f) = 0$. If $|y^r(x_f)|$ is smaller than a given tolerance of error ε_2, then the process of finding a solution is finished. Otherwise, we need to calculate the end values of $y(x_f)$ corresponding to a different $r_1 < r$ and $r_2 > r$, which are denoted by $y^{r_1}(x_f)$ and $y^{r_2}(x_f)$, respectively. If $y^{r_1}(x_f)y^r(x_f) < 0$, then there exists one root between r_1 and r; otherwise, the root is located between (r, r_2). Then, we may apply a half-interval method to find a suitable r, which requires us to calculate Eqs. (7)-(10) at each of the calculation of $y^r(x_f)$, until $|y^r(x_f)|$ is small enough to satisfy the criterion of $|y^r(x_f)| \le \varepsilon_2$.

In principle, we can increase the accuracy by imposing a smaller ε_2 on the shooting error, which however requires more iterations. Since the numerical method is very stable we can quickly pick up a correct value of r through some trials. Therefore, in the following calculations we do not use the above half-interval method to pick up the weighting factor r. When the best r is selected, we can use Eq. (72) to calculate A, such that the solution of y can be calculated.

We have mentioned that there are many solutions of the Sturm-Liouville eigenvalues problem. In order to give a unique solution we can consider the following normalized condition:

$$y'(x_0) = 1. \tag{76}$$

Therefore, in order to match the normalized condition (76) we can take the numerical solution of y by

$$y(x) = (x_f - x_0)\left[u - \frac{x - x_0}{x_f - x_0}\left(1 - \frac{x - x_0}{x_f - x_0}\right) - c\right] \Big/ (A - 1), \tag{77}$$

where u is calculated by the Lie-group shooting method. However, when $y'(x_0) = 0$ the above normalization cannot be used, and we can employ other normalization as to be shown by the following Example 3.

7 Numerical examples

7.1 *Example 1*

For a first and simple test example we consider the Sturm-Liouville eigenvalues problem with $x_0 = 0$, $x_f = \pi$, $p = s = 1$ and $q = 0$, and the solution is given by

$$y_k(x) = \sin kx, \quad k \in \mathbb{N}, \tag{78}$$

$$\lambda_k = k^2. \tag{79}$$

Here λ_k is the eigenvalue, and y_k is the eigenfunction.

We have applied the Lie-group shooting method in Section 5 to calculate the eigenvalues in a range of $8 < \lambda < 50$. From Fig. 1 it can be seen that the curve of $y(x_f)$ is intersected with the zero line at $\lambda = 9, 16, 25, 36, 49$, which are corresponding to $k = 3, 4, 5, 6, 7$. In this calculation the time stepsize used in the RK4 is $\Delta t = 0.0005$.

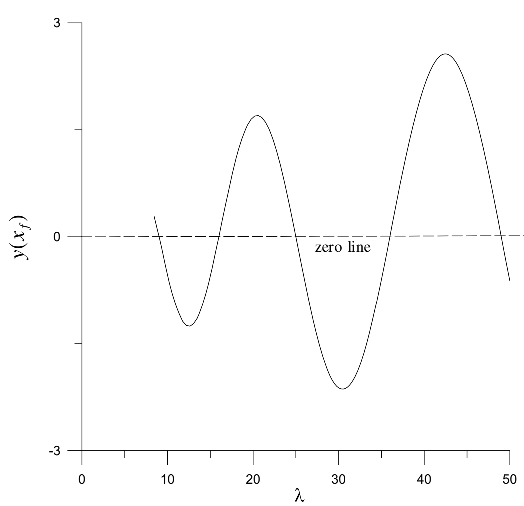

Figure 1: For Example 1 plotting the eigenvalues curve.

In Fig. 2 we compare the calculated eigenfunctions by using the Lie-group shooting method in Section 6 and the exact eigenfunctions for $k = 1, 3, 7$. It can be seen that the numerical errors are small. Without exception we have used a time stepsize $\Delta t = 0.001$ in the RK4 for the calculations of eigenfunctions.

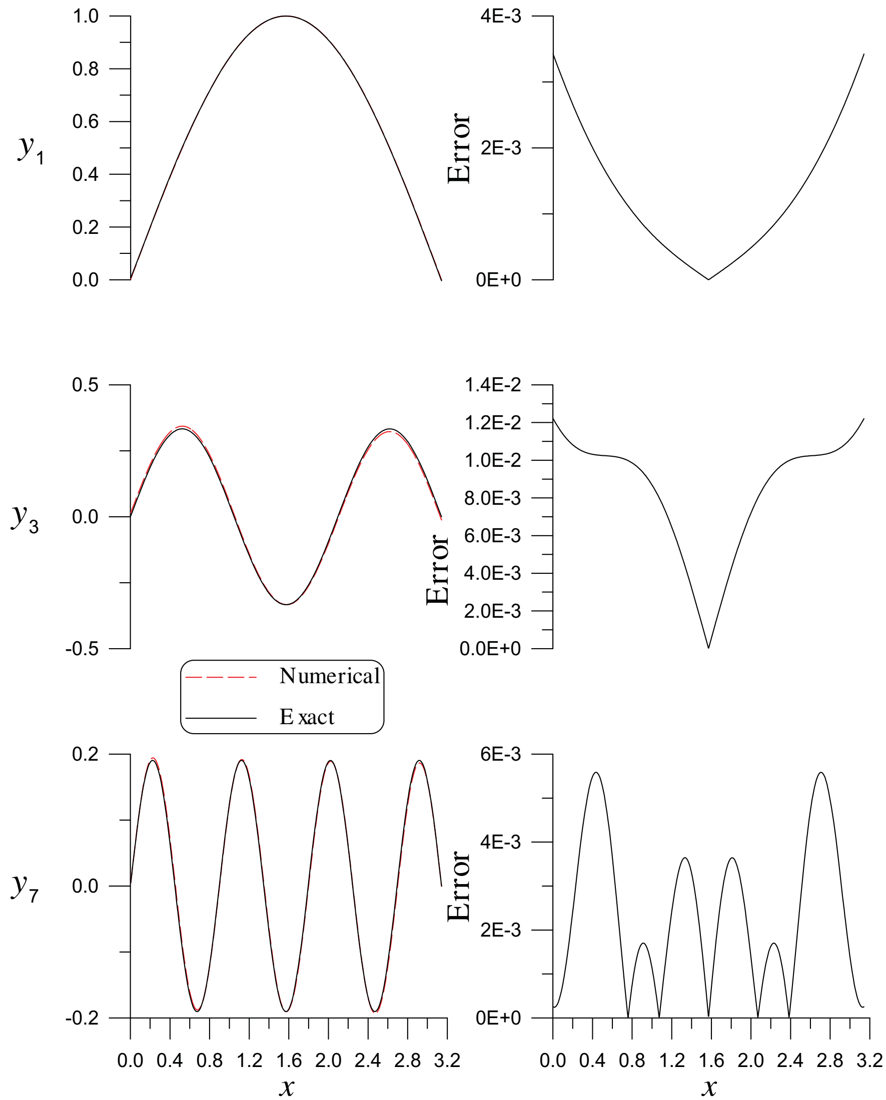

Figure 2: Comparing numerical and exact solutions for Example 1.

7.2 Example 2

For a second test example we consider the Sturm-Liouville eigenvalues problem with

$$[x^{-1}y'(x)]' + (\lambda+1)x^{-3}y(x) = 0, \tag{80}$$

$$y(1) = y(e) = 0. \tag{81}$$

The eigenvalue is $\lambda_k = k^2\pi^2$, $k \in \mathbb{N}$, and the eigenfunction is $y_k = x\sin(k\pi \ln x)$.

In Fig. 3 we compare the calculated eigenfunctions and exact eigenfunctions for $k = 1, 5, 10$. It can be seen that the numerical errors are small.

7.3 Example 3

For another test example we consider a singular Sturm-Liouville eigenvalues problem to calculate the eigenfunction in the Schrödinger equation

$$\frac{d^2y(x)}{dx^2} + (\lambda - x^2)y(x) = 0, \tag{82}$$

$$y(-\infty) = y(\infty) = 0. \tag{83}$$

Here $\lambda_k = 2k+1$, $k \in \mathbb{Z}^+$ is the eigenvalue, and

$$y_k(x) = H_k(x)\exp\left(-\frac{x^2}{2}\right) \tag{84}$$

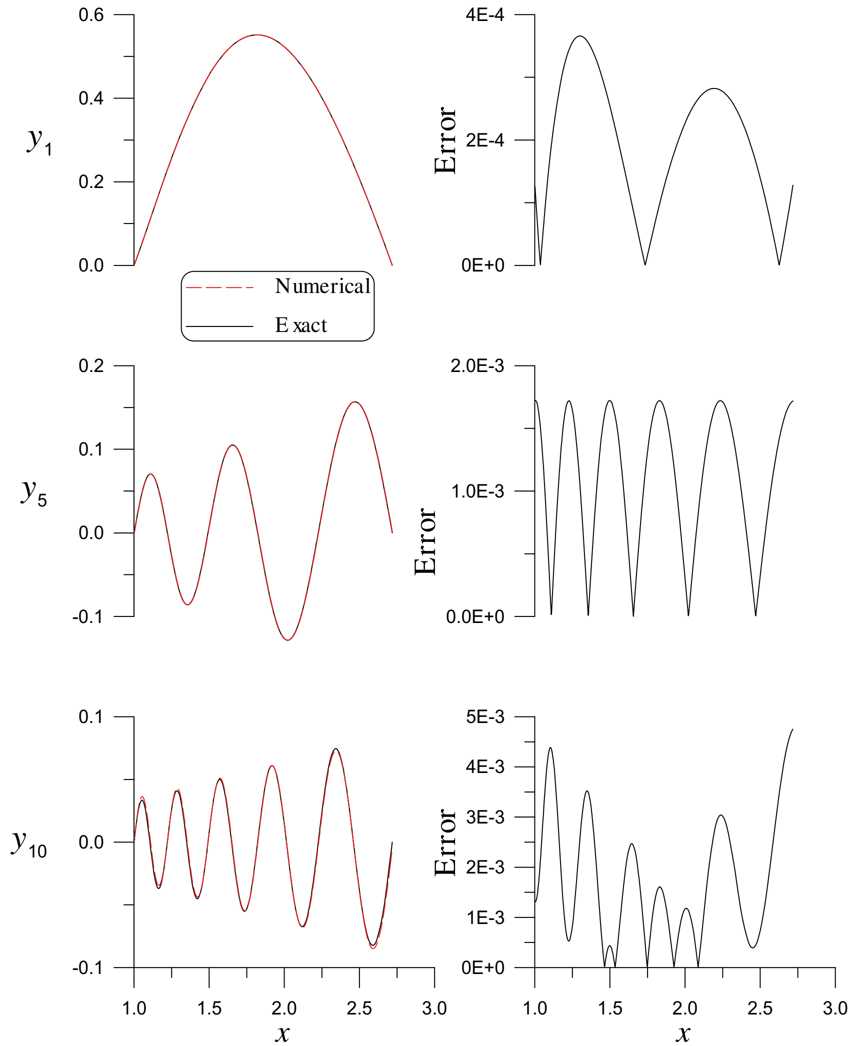

Figure 3: Comparing numerical and exact solutions for Example 2.

is the eigenfunction, where the Hermite polynomials for $k = 0, 1, 2, 3, 4$ are given by

$$H_0(x) = 1, \quad (85)$$

$$H_1(x) = 2x, \quad (86)$$

$$H_2(x) = -2 + 4x^2, \quad (87)$$

$$H_3(x) = -12x + 8x^3, \quad (88)$$

$$H_4(x) = 12 - 48x^2 + 16x^4. \quad (89)$$

In general, $H_k(x) = (-1)^k e^{x^2} d^k e^{-x^2}/dx^k$.

In Fig. 4 we compare the calculated eigenfunctions and exact eigenfunctions for $k = 2, 3, 4$ in the range of $-6 \leq x \leq 6$. The numerical errors are about in the order of 10^{-2}. The normalization employed for this example is by multiplying the numerical solution by a factor 2.

7.4 Example 4

For this example we consider the Sturm-Liouville eigenvalues problem with [Ghelardoni, Gheri and Marletta (2001); Yücel (2006)]:

$$-y''(x) + e^x y(x) = \lambda y(x), \quad (90)$$

$$y(0) = y(\pi) = 0. \quad (91)$$

The eigenvalue did not have a closed-form solution, and we first employed the Lie-group shooting method in Section 5 to search the eigenvalues in the range of $30 < \lambda < 920$ as shown in Fig. 5. There are 30 intersecting points of the eigenvalues curve with the zero line, which is coincident

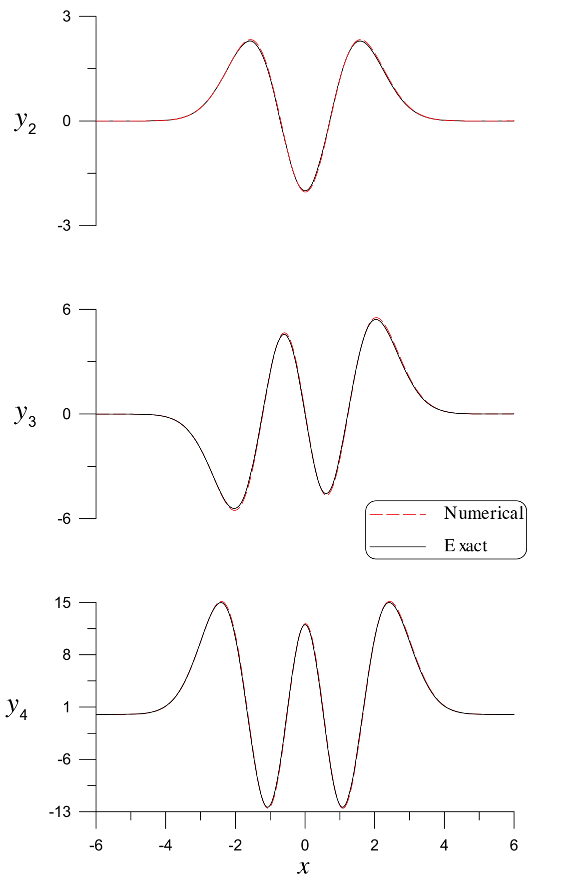

Figure 4: Comparing numerical and exact solutions for Example 3.

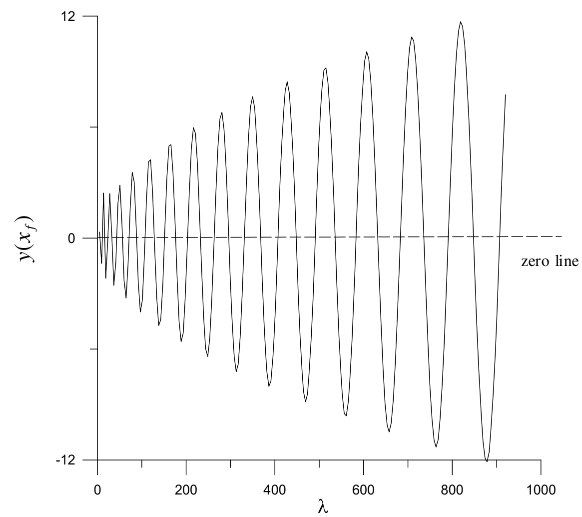

Figure 5: For Example 4 plotting the eigenvalues curve.

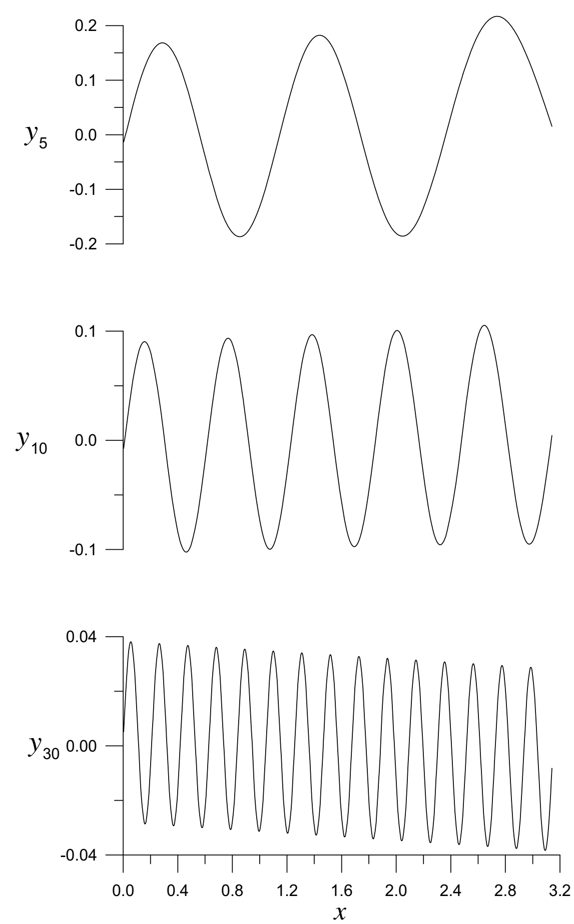

Figure 6: Computing the eigenfunctions for Example 4.

with that of the result given by Ghelardoni, Gheri and Marletta (2001). In Table 1 we compare our calculated eigenvalues through a finer adjusting of the eigenvalues to match the right-boundary condition $y(x_f) = 0$ with those by Ghelardoni, Gheri and Marletta (2001). In this calculation we were fixed $\Delta t = 10^{-4}$ and $\varepsilon_1 = 10^{-12}$. The last column also records the values of calculated $y(\pi)$ which is given by $y(\pi) = 0$ theoretically. When we use the eigenvalues provided by Ghelardoni, Gheri and Marletta (2001), we find that the right-boundary condition can be matched rather well with the accuracy in the order of 10^{-9}; however, our new eigenvalues can improve the accuracy at least three orders. We also calculate some eigenfunctions in Fig. 6 for $k = 5, 10, 30$.

Table 1: Comparing the eigenvalues for Example 4 with those of Ghelardoni, Gheri and Marletta (2001)

k	GGM's λ_k	present λ_k	$y(\pi)$
1	4.8966693800	4.89666937998	1.8×10^{-12}
5	32.263707046	32.263707045806	-2.4×10^{-13}
10	107.11667614	107.11667613843	4×10^{-13}
15	232.07881198	232.0788119867	3.4×10^{-12}
20	407.06523527	407.06523527773	-1.4×10^{-12}
25	632.05890789	632.0589079298	-3×10^{-12}
30	907.05546058	907.055460696755	-3.6×10^{-12}

7.5 Example 5

For the last example we consider another singular Sturm-Liouville eigenvalues problem with [Pryce (1993); Ghelardoni, Gheri and Marletta (2001)]:

$$-y''(x)+\left(x^2+\frac{3}{4x^2}\right)y(x)=\lambda y(x), \quad 0<x<\infty, \tag{92}$$

$$y(0)=y(\infty)=0, \tag{93}$$

which has theoretical eigenvalues $\lambda_k=4k,\ k\in\mathbb{N}$. As that done by Ghelardoni, Gheri and Marletta (2001) we replace the above problem by

$$-y''(x)+\left(x^2+\frac{3}{4x^2}\right)y(x)=\lambda y(x), \quad x_0<x<x_f, \tag{94}$$

$$y(x_0)=y(x_f^k)=0, \tag{95}$$

where we fix $x_0=0.0001$ and

$$x_f^k=4.0001\left(1+\frac{k-1}{10}\right),\ \ k\in\mathbb{N}. \tag{96}$$

In Table 2 we compare the errors of our calculated eigenvalues through a finer adjusting of the eigenvalues to match the right-boundary condition $y(x_f^k)=0$ with those by Ghelardoni, Gheri and Marletta (2001). In this calculation we have fixed $\Delta t=10^{-4}$. It can be seen that the accuracy is improved.

Table 2: Comparing the errors of eigenvalues for Example 5 with those of Ghelardoni, Gheri and Marletta (2001)

k	GGM's error	Present error
1	1.02×10^{-4}	9.95×10^{-5}
5	4.16×10^{-3}	4.15×10^{-3}
10	5.62×10^{-4}	5.40×10^{-4}
20	5.36×10^{-5}	3.30×10^{-7}
30	6.49×10^{-5}	4.60×10^{-7}
50	2.44×10^{-5}	5.06×10^{-6}
70	1.42×10^{-4}	9.10×10^{-6}

8 Conclusions

The new Lie-group shooting method developed here can be used to calculate the eigenvalues and eigenfunctions of Sturm-Liouville eigenvalues problems. The key point is relied on a closed-form formula of $A(\lambda)$ in the search of eigenvalues and $A(r)$ in the calculation of eigenfunctions. Several numerical examples 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 the past literature. And moreover the accuracy is improved significiantly.

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