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The Lie-Group Shooting Method for Nonlinear Two-Point Boundary Value Problems Exhibiting Multiple Solutions

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Summary

The present paper provides a Lie-group shooting method for the numerical solutions of second-order nonlinear boundary value problems exhibiting multiple solutions. It aims to find all solutions as easy as possible. The boundary conditions considered are classified into four types, namely the Dirichlet, the first Robin, the second Robin and the Neumann. The two Robin type problems are transformed into a canonical one by using the technique of symmetric extension of the governing equations. The Lie-group shooting method is very effective to search unknown initial condition through a weighting factor $r \in (0,1)$. Furthermore, the closed-form solutions are derived to calculate the unknown initial condition in terms of r in a more refined range identified. Numerical examples were examined to show that the new approach is highly efficient and accurate. The number of solutions can be identified in advance, and all possible solutions can be integrated readily through the obtained initial conditions by selecting suitable r.

keywords: Lie-group shooting method, Nonlinear boundary value problem, Unknown initial condition, Multiple solutions.

Introduction

In this paper we propose new method for the computations of the following second-order nonlinear boundary value problems (BVPs):

$$u'' = F(x,u,u'), \quad a < x < b, \tag{1}$$

where we consider four type boundary conditions with α and β given constants:

$$u(a) = \alpha, \quad u(b) = \beta, \tag{2}$$
$$u'(a) = \alpha, \quad u(b) = \beta, \tag{3}$$
$$u(a) = \alpha, \quad u'(b) = \beta, \tag{4}$$
$$u'(a) = \alpha, \quad u'(b) = \beta. \tag{5}$$

Eq. (1) together with Eq. (2) is called the Dirichlet type BVP, Eq. (1) together with Eq. (3) is called the first Robin type BVP, and Eq. (1) together with Eq. (4) is called the second Robin type BVP, while Eq. (1) together with Eq. (5) is called the Neumann type BVP. The last problem will be discussed until Section 8.

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The BVPs require information at a left-end point $x = a$ and at a right-end point $x = b$. For this reason the BVPs are also called the two-point boundary value problems (TPBVPs), which are often encountered in physical and engineering problems. A number of methods exist for solving these problems including shooting, collocation and finite difference methods. Among these methods the shooting method is the simplest one to solve TPBVPs. However, it is known that the shooting method may fail to converge for problems whose solutions are sensitive to initial guesses, or may be even unstable leading to large solution components that the solution does not extend until to the desired interval due to error in the initial guess. For this type problem finite difference and collocation methods can provide a solution that satisfies the boundary conditions and is close to the actual solution; however, the finite difference and collocation methods are much harder to set up than the shooting method. This led to the development of multiple shooting method as derived by Morrison, Riley and Zancanaro (1962), which is a compromise between the shooting method and the finite difference method. Keller (1992) refers to the multiple shooting method as parallel shooting.

The usual stepping scheme requires a complete information at the starting point $x = a$. Some effort is then required to reconcile the stepping scheme for the integrations of BVPs.

The shooting method is to assume some unknown initial conditions and to convert the BVP into initial value problem (IVP). Solve the IVP and compare the solution at the boundary to the known boundary conditions. In general, the solution will not immediately satisfy the boundary conditions, and, it requires many iterations to feedback the information of mismatch on the target defined by the boundary conditions to adjust the initial guess through iterative techniques. Thus the solution will converge to the desired boundary conditions by gradually varying the initial conditions. This iterative approach is called shooting method. How to choose a suitable initial condition may become difficult when the guesses are carried out in an uncertain range. The shooting method is a trial-and-error method and is often very sensitive to the initial guess. All that makes the computation expensive.

Especially, nonlinear BVPs often exhibit more than one solution for a given set of parameters. Because of this, by using the program with shooting method for solving nonlinear BVPs one requires to provide a guess for the solution desired. Along this way it is a difficult task to establish all possible solutions if more than one is expected. If the solutions are very close to each other, the shooting method fails to calculate the relevant profiles because of oscillation of a particular iteration procedure between both solutions.

Our approach of nonlinear BVPs is based on the group preserving scheme (GPS) developed by Liu (2001) for the integrations of IVPs. The GPS method is very effective to deal with ODEs with special structures as shown by Liu (2005, 2006a) for stiff equations and ODEs with constraints.

In this paper we will propose the Lie-group shooting method, which provides an analytical method to determine the unknown information at the starting point. It aims to make solving nonlinear BVPs even with multiple solutions as easy as possible. It will be clear that our method can be applied to the second-order nonlinear BVPs, since we are able to search the missing initial condition with closed-form solutions through r in a compact space of $r \in (0,1)$, where the factor r is used in a generalized mid-point rule for the Lie group of one-step GPS.

This paper is organized as follows. In Section 2 we put the first three type BVPs into a canonical form, where the symmetric extension techniques are used for the Robin type BVPs. In Section 3 we give a brief sketch of the group preserving scheme for ODEs and explain the construction of a one-step GPS by using the closure property of Lie group [Liu, Chang and Chang (2006), Liu (2006b)], and combine it with the generalized mid-point rule (mean value theorem) to construct a single-parameter Lie group in terms of the weighting factor r. In Section 4 we derive a Lie-group shooting method to solve nonlinear BVPs of the first three types, where we can search the missing initial condition by solving an algebraic equation in terms of r in a compact space of $r \in (0,1)$. In Section 5 we derive closed-form solutions of the missing initial condition in a more refined interval of r. In Section 6 we specify numerical procedures to adjusting the missing initial condition by a quick and correct pick of r. In Section 7 we use numerical examples to demonstrate the efficiency of the new method for the first three types BVPs. In Section 8 we derive the governing equations for the Neumann type BVPs and give a numerical example of this sort. Finally, we draw some conclusions in Section 9.

Transforming the BVPs into a canonical one

The Dirichlet type BVPs

By letting

$$x = a + (b-a)t, \tag{6}$$

$$y(t) = u(x) + (\alpha - \beta)t + c - \alpha, \tag{7}$$

we can transform Eqs. (1) and (2) into a mathematical equivalent system:

$$\ddot{y} = f_1(t, y, \dot{y}), \tag{8}$$

$$y(0) = c, \quad y(1) = c, \tag{9}$$

where $c > 0$ is a translation constant. The superimposed dot denotes the differential with respect to t. Here, we let

$$f_1(t,y,\dot{y}) := (b-a)^2 F(a + (b-a)t, y + (\beta - \alpha)t + \alpha - c, (\dot{y} + \beta - \alpha)/(b-a)). \tag{10}$$

The first Robin type BVPs

In addition Eq. (6) we use the following transformation:

$$y(t) = u(x) + \alpha(b-a)(1-t) + c - \beta, \tag{11}$$

and then Eqs. (1) and (3) can be reduced to

$$\ddot{y} = F_1(t, y, \dot{y}), \tag{12}$$

$$\dot{y}(0) = 0, \quad y(1) = c, \tag{13}$$

where

$$F_1(t, y, \dot{y}) := (b-a)^2 F(a + (b-a)t, y + \alpha(a-b)(1-t) + \beta - c, \dot{y}/(b-a) + \alpha). \tag{14}$$

Through a symmetric extension into the interval of $t \in [-1, 0)$, we can write Eqs. (12) and (13) to be

$$\ddot{y} = f_2(t, y, \dot{y}), \tag{15}$$

$$y(-1) = c, \quad y(1) = c, \tag{16}$$

where

$$f_2(t, y, \dot{y}) = \begin{cases} F_1(t, y, \dot{y}) & \text{if} \quad 0 \le t \le 1, \\ F_1(-t, y, -\dot{y}) & \text{if} \quad -1 \le t < 0. \end{cases} \tag{17}$$

The condition $\dot{y}(0) = 0$ will be not imposed here until we develop the shooting method in Sections 4-6.

The second Robin type BVPs

For Eqs. (1) and (4) we consider the following transformations:

$$x = b + (b-a)t, \tag{18}$$

$$y(t) = u(x) - \beta(b-a)(1+t) + c - \alpha, \tag{19}$$

such that

$$\ddot{y} = F_2(t, y, \dot{y}), \tag{20}$$

$$y(-1) = c, \quad \dot{y}(0) = 0, \tag{21}$$

where

$$F_2(t, y, \dot{y}) := (b-a)^2 F(b + (b-a)t, y + \beta(b-a)(1+t) + \alpha - c, \dot{y}/(b-a) + \beta). \tag{22}$$

Through a symmetric extension into the interval of $t \in (0,1]$, we can write Eqs. (20) and (21) to be

$$\ddot{y} = f_3(t,y,\dot{y}), \tag{23}$$

$$y(-1) = c, \quad y(1) = c, \tag{24}$$

where

$$f_3(t,y,\dot{y}) = \begin{cases} F_2(-t,y,-\dot{y}) & \text{if} \quad 0 < t \leq 1, \\ F_2(t,y,\dot{y}) & \text{if} \quad -1 \leq t \leq 0. \end{cases} \tag{25}$$

The canonical form

The first three type BVPs are all transformed into the same type BVP:

$$\ddot{y} = f(t,y,\dot{y}), \tag{26}$$

$$y(t_0) = c, \quad y(1) = c, \tag{27}$$

but with different f and t_0. The case with $t_0 = 0$ and $f = f_1$ corresponds to the Dirichlet type BVP, and $t_0 = -1$ and $f = f_2$ to the first Robin type BVP, while $t_0 = -1$ and $f = f_3$ to the second Robin type BVP. No matter which type BVP is considered, we can treat these equations in a unified manner by starting from Eqs. (26) and (27).

For the latter two types BVPs the integration must match the condition $\dot{y}(0) = 0$. Then, the solution of the original first Robin type BVP is obtained by taking the right-branch of the solution of Eqs. (26) and (27) with f replaced by f_2. Similarly, the solution of the original second Robin type BVP is obtained by taking the left-branch of the solution of Eqs. (26) and (27) with f replaced by f_3. In the later it would be appreciated the advantage by transforming the original BVPs to the standard type BVP in Eqs. (26) and (27) by enforcing the two boundary values identical.

The stepping techniques developed for IVPs require the initial conditions of both $y_1 = y$ and $y_2 = \dot{y}$ for the second-order ODEs. If the initial value of y_2, denoted as $y_2(t_0) = A$, is available, which together with the known initial value of $y_1(t_0) = c$, then we can numerically integrate the following IVP step-by-step in a forward direction from $t = t_0$ to $t = 1$:

$$\dot{y}_1 = y_2, \tag{28}$$

$$\dot{y}_2 = f(t,y_1,y_2), \tag{29}$$

$$y_1(t_0) = c, \tag{30}$$

$$y_2(t_0) = A. \tag{31}$$

Here, we call Eqs. (28)-(31) the $(\mathbf{y},t)$-IVP, where $\mathbf{y}(t)=(y_1(t),y_2(t))$ denotes the system variables in the t-domain. We are going to develop a Lie-group shooting method to solve A. If y in terms of t is available, then the solution of u in the x-domain can be obtained through Eqs. (6) and (7) for the Dirichlet problem, Eqs. (6) and (11) for the first Robin problem, and Eqs. (18) and (19) for the second Robin problem.

One-step GPS

The GPS

Let us write Eqs. (28) and (29) in the vector form:

$$\dot{\mathbf{y}}=\mathbf{f}(t,\mathbf{y}), \tag{32}$$

where

$$\mathbf{y}:=\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}, \quad \mathbf{f}:=\begin{bmatrix} y_2 \\ f(t,y_1,y_2) \end{bmatrix}. \tag{33}$$

Liu (2001) has embedded Eq. (32) into an augmented system:

$$\dot{\mathbf{X}}:=\frac{d}{dt}\begin{bmatrix} \mathbf{y} \\ \|\mathbf{y}\| \end{bmatrix}=\begin{bmatrix} \mathbf{0}_{2\times 2} & \frac{\mathbf{f}(t,\mathbf{y})}{\|\mathbf{y}\|} \\ \frac{\mathbf{f}^{\mathrm{T}}(t,\mathbf{y})}{\|\mathbf{y}\|} & 0 \end{bmatrix}\begin{bmatrix} \mathbf{y} \\ \|\mathbf{y}\| \end{bmatrix}:=\mathbf{A}\mathbf{X}, \tag{34}$$

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

$$\mathbf{A}^{\mathrm{T}}\mathbf{g}+\mathbf{g}\mathbf{A}=\mathbf{0} \tag{35}$$

with

$$\mathbf{g}=\begin{bmatrix} \mathbf{I}_2 & \mathbf{0}_{2\times 1} \\ \mathbf{0}_{1\times 2} & -1 \end{bmatrix} \tag{36}$$

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

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

$$\mathbf{X}^{\mathrm{T}}\mathbf{g}\mathbf{X}=\mathbf{y}\cdot\mathbf{y}-\|\mathbf{y}\|^2=0. \tag{37}$$

Accordingly, Liu (2001) has developed a group-preserving scheme (GPS) to guarantee that each $\mathbf{X}_k$ is located on the cone:

$$\mathbf{X}_{k+1}=\mathbf{G}(k)\mathbf{X}_k, \tag{38}$$

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

$$\mathbf{G}^{\mathrm{T}}\mathbf{g}\mathbf{G}=\mathbf{g}, \tag{39}$$

$$\det\mathbf{G}=1, \tag{40}$$

$$G_0^0>0, \tag{41}$$

where G_0^0 is the 00th component of $\mathbf{G}$. In Section 6.1 we will write the GPS explicitly.

Generalized mid-point rule

Applying scheme (38) to Eq. (34) with a specified initial condition $\mathbf{X}(t_0) = \mathbf{X}_0$ we can compute the solution $\mathbf{X}(t)$ by GPS. Assuming that the stepsize used in GPS is $h = (1-t_0)/K$, and starting from an initial augmented condition $\mathbf{X}_0 = \mathbf{X}(t_0) = (\mathbf{y}_0^{\mathrm{T}}, \|\mathbf{y}_0\|)^{\mathrm{T}}$ we will calculate the value $\mathbf{X}(1) = (\mathbf{y}^{\mathrm{T}}(1), \|\mathbf{y}(1)\|)^{\mathrm{T}}$ at $t = 1$.

By applying Eq. (38) step-by-step we can obtain

$$\mathbf{X}_f = \mathbf{G}_K(h)\cdots\mathbf{G}_1(h)\mathbf{X}_0, \tag{42}$$

where $\mathbf{X}_f$ approximates the exact $\mathbf{X}(1)$ with a certain accuracy depending on h. 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, $\mathbf{G}_K(h)\cdots\mathbf{G}_1(h)$ is also a Lie group denoted by $\mathbf{G}$. Hence, we have

$$\mathbf{X}_f = \mathbf{G}\mathbf{X}_0. \tag{43}$$

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

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 $\mathbf{A} \in so(2,1)$ by an exponential admits a closed-form representation as follows:

$$\mathbf{G} = \begin{bmatrix} \mathbf{I}_2 + \frac{(a-1)}{\|\hat{\mathbf{f}}\|^2}\hat{\mathbf{f}}\hat{\mathbf{f}}^{\mathrm{T}} & \frac{b\hat{\mathbf{f}}}{\|\hat{\mathbf{f}}\|} \\ \frac{b\hat{\mathbf{f}}^{\mathrm{T}}}{\|\hat{\mathbf{f}}\|} & a \end{bmatrix}, \tag{44}$$

where

$$\hat{\mathbf{y}} = r\mathbf{y}_0 + (1-r)\mathbf{y}_f, \tag{45}$$

$$\hat{\mathbf{f}} = \mathbf{f}(\hat{t}, \hat{\mathbf{y}}), \tag{46}$$

$$a = \cosh\left((1-t_0)\frac{\|\hat{\mathbf{f}}\|}{\|\hat{\mathbf{y}}\|}\right), \tag{47}$$

$$b = \sinh\left((1-t_0)\frac{\|\hat{\mathbf{f}}\|}{\|\hat{\mathbf{y}}\|}\right). \tag{48}$$

Here, we use the initial $\mathbf{y}_0 = (y_1(t_0), y_2(t_0))$ and the final $\mathbf{y}_f = (y_1(1), y_2(1))$ through a suitable weighting factor r to calculate $\mathbf{G}$, where $r \in (0,1)$ is a parameter and $\hat{t} = t_0 + r(1-t_0)$.

The approach of Eq. (44) can be realized alternatively by using

$$\dot{\mathbf{G}} = \mathbf{A}(t, \mathbf{y})\mathbf{G}. \tag{49}$$

Integrating the above equation and using the mean-value theorem we obtain

$$\mathbf{G} = \exp\left[\int_{t_0}^{1} \mathbf{A}(t, \mathbf{y})dt\right] = \exp[(1-t_0)\mathbf{A}(\hat{t}, \hat{\mathbf{y}})]. \tag{50}$$

Inserting Eq. (34) for $\mathbf{A}$ and calculating the exponential we can derive Eq. (44) again.

The above methods applied a generalized mid-point rule or the mean value theorem on the calculations of $\mathbf{G}$, and the resultant is a single-parameter Lie group element denoted by $\mathbf{G}(r)$.

A Lie group mapping between two points on the cone

Let us define a new vector

$$\mathbf{F} := \frac{\hat{\mathbf{f}}}{\|\hat{\mathbf{y}}\|}, \tag{51}$$

such that Eqs. (44), (47) and (48) can also be expressed as

$$\mathbf{G} = \begin{bmatrix} \mathbf{I}_2 + \frac{a-1}{\|\mathbf{F}\|^2}\mathbf{F}\mathbf{F}^{\mathrm{T}} & \frac{b\mathbf{F}}{\|\mathbf{F}\|} \\ \frac{b\mathbf{F}^{\mathrm{T}}}{\|\mathbf{F}\|} & a \end{bmatrix}, \tag{52}$$

$$a = \cosh[(1-t_0)\|\mathbf{F}\|], \tag{53}$$

$$b = \sinh[(1-t_0)\|\mathbf{F}\|]. \tag{54}$$

From Eqs. (43) and (52) it follows that

$$\mathbf{y}_f = \mathbf{y}_0 + \eta\mathbf{F}, \tag{55}$$

$$\|\mathbf{y}_f\| = a\|\mathbf{y}_0\| + b\frac{\mathbf{F}\cdot\mathbf{y}_0}{\|\mathbf{F}\|}, \tag{56}$$

where

$$\eta := \frac{(a-1)\mathbf{F}\cdot\mathbf{y}_0 + b\|\mathbf{y}_0\|\|\mathbf{F}\|}{\|\mathbf{F}\|^2}. \tag{57}$$

Substituting

$$\mathbf{F} = \frac{1}{\eta}(\mathbf{y}_f - \mathbf{y}_0) \tag{58}$$

obtained from Eq. (55), into Eq. (56) we obtain

$$\frac{\|\mathbf{y}_f\|}{\|\mathbf{y}_0\|} = a + b\frac{(\mathbf{y}_f - \mathbf{y}_0)\cdot\mathbf{y}_0}{\|\mathbf{y}_f - \mathbf{y}_0\|\|\mathbf{y}_0\|}, \tag{59}$$

where

$$a=\cosh\left(\frac{(1-t_0)\|\mathbf{y}_f-\mathbf{y}_0\|}{\eta}\right), \tag{60}$$

$$b=\sinh\left(\frac{(1-t_0)\|\mathbf{y}_f-\mathbf{y}_0\|}{\eta}\right) \tag{61}$$

are obtained by inserting Eq. (58) for **F** into Eqs. (53) and (54).

Let

$$\cos\theta := \frac{[\mathbf{y}_f-\mathbf{y}_0]\cdot\mathbf{y}_0}{\|\mathbf{y}_f-\mathbf{y}_0\|\|\mathbf{y}_0\|}, \tag{62}$$

$$S := (1-t_0)\|\mathbf{y}_f-\mathbf{y}_0\|, \tag{63}$$

and from Eqs. (59)-(61) it follows that

$$\frac{\|\mathbf{y}_f\|}{\|\mathbf{y}_0\|}=\cosh\left(\frac{S}{\eta}\right)+\cos\theta\sinh\left(\frac{S}{\eta}\right). \tag{64}$$

By defining

$$Z:=\exp\left(\frac{S}{\eta}\right), \tag{65}$$

we obtain a quadratic equation for Z from Eq. (64):

$$(1+\cos\theta)Z^2-\frac{2\|\mathbf{y}_f\|}{\|\mathbf{y}_0\|}Z+1-\cos\theta=0. \tag{66}$$

The solution is found to be

$$Z=\frac{\frac{\|\mathbf{y}_f\|}{\|\mathbf{y}_0\|}+\sqrt{\left(\frac{\|\mathbf{y}_f\|}{\|\mathbf{y}_0\|}\right)^2-1+\cos^2\theta}}{1+\cos\theta}, \tag{67}$$

and then from Eqs. (65) and (63) we obtain

$$\eta=\frac{(1-t_0)\|\mathbf{y}_f-\mathbf{y}_0\|}{\ln Z}. \tag{68}$$

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

$$\begin{bmatrix}\mathbf{y}_f\\ \|\mathbf{y}_f\|\end{bmatrix}=\mathbf{G}\begin{bmatrix}\mathbf{y}_0\\ \|\mathbf{y}_0\|\end{bmatrix}, \tag{69}$$

where $\mathbf{G}$ is uniquely determined by $\mathbf{y}_0$ and $\mathbf{y}_f$ through the following equations:

$$\mathbf{G}(\mathbf{y}_0,\mathbf{y}_f) = \begin{bmatrix} \mathbf{I}_2 + \frac{a-1}{\|\mathbf{F}\|^2}\mathbf{F}\mathbf{F}^{\mathrm{T}} & \frac{b\mathbf{F}}{\|\mathbf{F}\|} \\ \frac{b\mathbf{F}^{\mathrm{T}}}{\|\mathbf{F}\|} & a \end{bmatrix}, \tag{70}$$

$$a = \cosh[(1-t_0)\|\mathbf{F}\|], \tag{71}$$

$$b = \sinh[(1-t_0)\|\mathbf{F}\|], \tag{72}$$

$$\mathbf{F} = \frac{1}{\eta}(\mathbf{y}_f - \mathbf{y}_0), \tag{73}$$

in which η is still calculated by Eq. (68).

It should be stressed that the above $\mathbf{G}$ is very different from the one in Eq. (44). In order to feature its dependence only on $\mathbf{y}_0$ and $\mathbf{y}_f$, we write it to be $\mathbf{G}(\mathbf{y}_0,\mathbf{y}_f)$, which is independent on r. Converesely, the r-dependence $\mathbf{G}(r)$ is also a function of $\mathbf{y}_0$ and $\mathbf{y}_f$, but its dependence is through the vector field $\mathbf{f}$ and the mean values of $\hat{\mathbf{y}}$. However, that two Lie group elements $\mathbf{G}(r)$ and $\mathbf{G}(\mathbf{y}_0,\mathbf{y}_f)$ are both indispensable in our development of the Lie-group shooting method for nonlinear BVPs.

The Lie-group shooting method

From Eqs. (28)-(31) it follows that

$$\dot{y}_1 = y_2, \tag{74}$$

$$\dot{y}_2 = f(t,y_1,y_2), \tag{75}$$

$$y_1(t_0) = c, \quad y_1(1) = c, \tag{76}$$

$$y_2(t_0) = A, \quad y_2(1) = B, \tag{77}$$

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

From Eqs. (73), (76) and (77) it follows that

$$\mathbf{F} := \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} = \frac{1}{\eta}\begin{bmatrix} 0 \\ B-A \end{bmatrix}. \tag{78}$$

From Eqs. (68), (67) and (62) by inserting Eq. (33) for $\mathbf{y}$ and noting that

$$\mathbf{y}_0 = \begin{bmatrix} c \\ A \end{bmatrix}, \quad \mathbf{y}_f = \begin{bmatrix} c \\ B \end{bmatrix}, \tag{79}$$

we obtain

$$\eta = \frac{(1-t_0)\sqrt{(A-B)^2}}{\ln Z}, \tag{80}$$

$$Z = \frac{\frac{\sqrt{c^2+B^2}}{\sqrt{c^2+A^2}} + \sqrt{\frac{c^2+B^2}{c^2+A^2} - 1 + \cos^2\theta}}{1+\cos\theta}, \tag{81}$$

$$\cos\theta = \frac{A(B-A)}{\sqrt{(A-B)^2}\sqrt{c^2+A^2}}. \tag{82}$$

When compare Eq. (78) with Eq. (51), and with the aid of Eqs. (45), (46) and (74)-(77) we obtain

$$rA + (1-r)B = 0, \tag{83}$$

$$A - B + \frac{\eta}{\xi}\hat{f} = 0, \tag{84}$$

where

$$\hat{f}(r) := f(t_0 + r(1-t_0), c, 0), \tag{85}$$

$$\xi := \sqrt{c^2 + [rA + (1-r)B]^2}. \tag{86}$$

It can be seen that $\hat{f}$ is simply a function of r. This result is due to the fact of $\hat{y}_1 = rc + (1-r)c = c$ and $\hat{y}_2 = rA + (1-r)B = 0$ by Eqs. (76), (77) and (83). Of course, this is our objective to reduce the governing equation with its most simple form, which is due to the fact that we have transformed the BVPs into a canonical one in Eq. (26) with the two boundary values in Eq. (27) identical.

The above derivation of the governing equations (80)-(86) is based on by equating the two **F**'s in Eqs. (51) and (73). It also means that the two Lie group elements defined by Eqs. (44) and (70) are equal. In this sense we may call our shooting technique a *Lie-group shooting method*.

From Eqs. (83) and (86) it follows that

$$\xi = c, \tag{87}$$

which is a positive constant. Hence, from Eqs. (83)-(85) and (87) we obtain a single algebraic equation for the unknown variable A:

$$Ac + \eta_0 \hat{f} = 0, \tag{88}$$

where

$$Z = \frac{\sqrt{c^2+B^2}+\sqrt{B^2}}{\sqrt{c^2+A^2}-\sqrt{A^2}}, \tag{89}$$

$$\eta_0 = \frac{(1-t_0)\sqrt{A^2}}{\ln Z}, \tag{90}$$

and $B = rA/(r-1)$ has a different sign with A.

Eq. (88) can be used to solve A for a given r. If A is available, we can return to integrate Eqs. (28)-(31) by a suitable forward IVP solver.

The solution of A

Remarkably, Eq. (88) can be solved exactly for A.

The case of $A > 0$

Here we first consider the case of $A > 0$. Inserting Eq. (90) for η_0 into Eq. (88) we obtain

$$\ln Z = \frac{-(1-t_0)\hat{f}}{c}. \tag{91}$$

Defining

$$g_1 := \exp\left(-\frac{(1-t_0)\hat{f}}{c}\right), \tag{92}$$

and substituting Eq. (89) for Z into Eq. (91) we obtain

$$\frac{\sqrt{c^2+B^2}+\sqrt{B^2}}{\sqrt{c^2+A^2}-\sqrt{A^2}} = g_1. \tag{93}$$

Eq. (93) can be written as

$$g_1 A - B = g_1\sqrt{c^2+A^2} - \sqrt{c^2+B^2}, \tag{94}$$

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

$$2g_1\sqrt{c^2+B^2}\sqrt{c^2+A^2} = (1+g_1^2)c^2 + 2g_1 AB. \tag{95}$$

Squaring again and cancelling the common term and factor we get

$$4g_1^2(A^2+B^2) - 4g_1(1+g_1^2)AB = (1-g_1^2)^2c^2. \tag{96}$$

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

$$\frac{4g_1}{(r-1)^2}[-(1-g_1)^2r^2 + (1-g_1)^2 r + g_1]A^2 = (1-g_1^2)^2c^2. \tag{97}$$

If the following condition holds

$$D_1(r) := -(1-g_1)^2 r^2 + (1-g_1)^2 r + g_1 > 0, \tag{98}$$

then A has a positive solution:

$$A = \sqrt{\frac{(r-1)^2(1-g_1^2)^2 c^2}{4D_1 g_1}}. \tag{99}$$

The discriminant function $D_1(r)$ is an open-down distorted parabola of r since g_1 is also a function of r. $D_1(r)$ has the following properties:

$$D_1(0) = D_1(1) = g_1, \tag{100}$$

and there exist two roots of r for $D_1(r) = 0$:

$$r_1 = \frac{1}{2} - \frac{1+g_1}{2(1-g_1)} = \frac{-g_1}{1-g_1}, \quad r_2 = \frac{1}{2} + \frac{1+g_1}{2(1-g_1)} = \frac{1}{1-g_1}. \tag{101}$$

The condition (98) can be used to detect the range where r is permitted.

The case of $A < 0$

Next we consider the case of $A < 0$. Inserting Eq. (90) for η_0 into Eq. (88) we obtain:

$$\ln Z = \frac{(1-t_0)\hat{f}}{c}. \tag{102}$$

Defining

$$g_2 := \exp\left(\frac{(1-t_0)\hat{f}}{c}\right), \tag{103}$$

and substituting Eq. (89) for Z into Eq. (102) we obtain

$$\frac{\sqrt{c^2+B^2}+\sqrt{B^2}}{\sqrt{c^2+A^2}-\sqrt{A^2}} = g_2. \tag{104}$$

By using $A < 0$ and $B > 0$, Eq. (104) can be written as

$$g_2 A + B = \sqrt{c^2+B^2} - g_2\sqrt{c^2+A^2}. \tag{105}$$

Squaring the above equation and cancelling the common terms we can rearrange it to

$$2g_2\sqrt{c^2+B^2}\sqrt{c^2+A^2} = (1+g_2^2)c^2 - 2g_2 AB. \tag{106}$$

Squaring again and cancelling the common term and factor we get

$$4g_2^2(A^2+B^2)+4g_2(1+g_2^2)AB=(1-g_2^2)^2c^2. \tag{107}$$

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

$$\frac{4g_2}{(r-1)^2}[(1+g_2)^2r^2-(1+g_2)^2r+g_2]A^2=(1-g_2^2)^2c^2. \tag{108}$$

If the following condition holds

$$D_2(r) := (1+g_2)^2r^2-(1+g_2)^2r+g_2>0, \tag{109}$$

then A has a negative solution:

$$A=-\sqrt{\frac{(r-1)^2(1-g_2^2)^2c^2}{4D_2g_2}}. \tag{110}$$

The discriminant function $D_2(r)$ is an open-up distorted parabola of r since g_2 is also a function of r. By inspection, $D_2(r)$ has the following properties:

$$D_2(0)=D_2(1)=g_2, \tag{111}$$

and there exist two roots of r for $D_2(r)=0$:

$$r_1=\frac{1}{2}-\frac{g_2-1}{2(g_2+1)}=\frac{1}{g_2+1}, \quad r_2=\frac{1}{2}+\frac{g_2-1}{2(g_2+1)}=\frac{g_2}{g_2+1}, \tag{112}$$

where $0 < r_1 < 0.5 < r_2 < 1$. There exist solutions of A given by Eq. (110) in the following ranges of r:

$$0<r<r_1, \quad r_2<r<1. \tag{113}$$

Adjusting the slope A

In the previous section we have derived the closed-form solution to calculate the slope A for each r in its admissible range. If A is available, then we can apply the GPS method given below to integrate the $(\mathbf{y},t)$-IVP in Eqs. (28)-(31). Up to this point we should note that the Lie-group shooting method is an exactly solving technique for the second-order nonlinear BVPs without making any assumption or the approximation in the derivations of all required formulas. However, how to determine a correct r and thus A requires a numerical integration of the nonlinear ODEs.

The GPS

We have derived the closed-form solutions to calculate the slope A for each r in its admissible range, and thus we can integrate the $(\mathbf{y},t)$-IVP in Eqs. (28)-(31) by the following GPS method:

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \frac{4\|\mathbf{y}_n\|^2 + 2h\mathbf{f}_n \cdot \mathbf{y}_n}{4\|\mathbf{y}_n\|^2 - h^2\|\mathbf{f}_n\|^2} h\mathbf{f}_n, \tag{114}$$

where

$$\mathbf{f}_n = \mathbf{f}(t_n, \mathbf{y}_n). \tag{115}$$

The numerical scheme (114) was first derived by Liu (2001).

Adjusting *A* for the Dirichlet type BVPs

For a trial r in the admissible range, we can calculate A and then numerically integrate Eqs. (28)-(31) from $t = 0$ to $t = 1$, and compare the end value of $y_1^r(1)$ with the exact one $y_1(1) = c$. If $|y_1^r(1) - c|$ is smaller than a given error tolerance ε, then the process of finding solution is finished. Otherwise, we need to calculate the end values of $y_1(1)$ corresponding to different $r_1 < r$ and $r_2 > r$, which are denoted by $y_1^{r_1}(1)$ and $y_1^{r_2}(1)$, respectively. If $[y_1^{r_1}(1) - c][y_1^r(1) - c] < 0$, then there exists one root between r_1 and r; otherwise, the root is located between (r, r_2). Then, we apply the half-interval method to find a suitable r, which requires us to calculate Eqs. (28)-(31) at each of the calculation of $y_1^r(1) - c$, until $|y_1^r(1) - c|$ is small enough to satisfy the criterion of $|y_1^r(1) - c| \le \varepsilon$.

Adjusting *A* for the Robin type BVPs

For the first and second Robin type BVPs, we have employed the symmetric extension techniques to construct the canonical equations. Therefore the target used to adjust the slope A is $\dot{y}(0) = 0$.

For a trial r in the admissible range, we can calculate A and then numerically integrate Eqs. (28)-(31) from $t = -1$ to $t = 0$, and compare the end value of $y_2^r(0)$ with the exact one $y_2(0) = \dot{y}(0) = 0$. If $|y_2^r(0)|$ is smaller than ε, then the process of finding solution is finished. Otherwise, we need to calculate the end values of $y_2(0)$ corresponding to different $r_1 < r$ and $r_2 > r$, which are denoted by $y_2^{r_1}(0)$ and $y_2^{r_2}(0)$, respectively. If $y_2^{r_1}(0)y_2^r(0) < 0$, then there exists one root between r_1 and r; otherwise, the root is located between (r, r_2). Then, we apply the half-interval method to find a suitable r, which requires us to calculate Eqs. (28)-(31) at each of the calculation of $y_2^r(0)$, until $|y_2^r(0)|$ is small enough to satisfy the criterion of $|y_2^r(0)| \le \varepsilon$.

In principle, we can increase the accuracy by imposing a smaller ε on the shooting error, which however requires more iterations. Since the numerical method is very stable we can quickly pick up the correct value of r through some trials and modifications. Therefore, in the following calculations of numerical examples we do not use the above half-interval method to pick up the weighting factor r.

Numerical examples

Example 1

Let us consider the following BVP (Ha and Lee, 2001):

$$u'' = \frac{3}{2}u^2, \tag{116}$$

$$u(0) = 4, \quad u(1) = 1. \tag{117}$$

The exact solution is

$$u(x) = \frac{4}{(1+x)^2}. \tag{118}$$

It needs to stress that the solution of Eq. (116) is not unique. In addition the above one, there exists another solution:

$$u(x) = c_1^2 \left(\frac{1-\mathrm{cn}(c_1x - c_2, k^2)}{1+\mathrm{cn}(c_1x - c_2, k^2)} - \frac{1}{\sqrt{3}} \right), \tag{119}$$

where $\mathrm{cn}(\xi, k)$ is the modulus k Jacobi elliptic function. In the above case we have $c_1 = 4.30310990$, $c_2 = 2.3346196$, and $k = \sqrt{2+\sqrt{3}}/2$.

In this problem the vector field $F = 3u^2/2$ cannot satisfy the unique conditions of BVP, since $\partial F/\partial u = 3u$ may be negative, for example the solution in Eq. (119). On the other hand, since F may be zero when u passes the zero axis, we consider a translation of u in Eq. (116) by Eq. (7), such that one has

$$\ddot{y} = \frac{3}{2}[y - 3t + 4 - c]^2, \tag{120}$$

$$y(0) = c, \quad y(1) = c. \tag{121}$$

Then we apply the method in Sections 4-6 on the above equation, and then obtain u by $u = y - 3t + 4 - c$.

For each given r we use Eq. (110) to calculate A, and then numerically integrate the IVP by the numerical scheme in Section 6.1. We plot the curve of A with respect to r in Fig. 1(a), and the curve of $y_1(1) - c$ with respect to r in Fig. 1(b). In this calculation we have fixed $c = 15$ and the stepsize $h = 0.0001$. It can be seen that there are two roots of r, of which the target equation $y_1(1) - c = 0$ is satisfied as shown in Fig. 1(b) at the intersection points of the curve with the zero line.

Then, we apply the Lie-group shooting technique to this problem for searching the missing initial condition $y_2(0) = A$. In Fig. 2 we compare our solutions with the exact solutions by taking $r = 0.69334382$ for smaller solution and $r = 0.61959981$

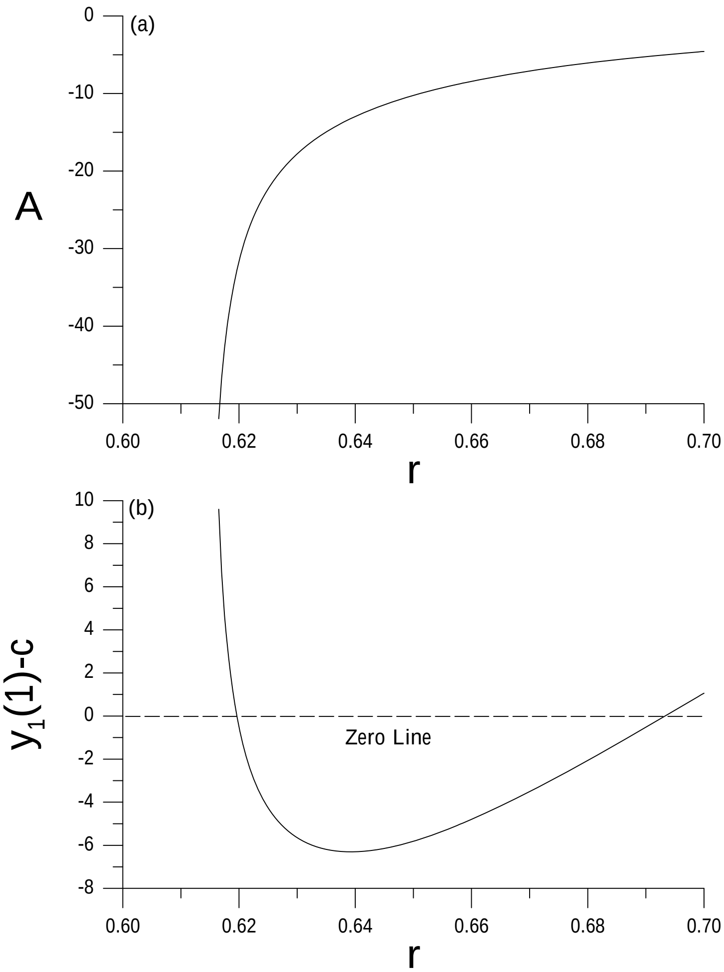

Figure 1: For Example 1 we plot A with respect to r in (a), and $y_1(1) - c$ with respect to r in (b), where the intersection points locate the roots of r.

for larger solution. They lead to the errors of the value of $y_1(1)$ in the order of 10^{-7} when compared with the exact $y_1(1) = c$. We only compare our solution with the solution in Eq. (118), which is the smaller one. It can be seen that the numerical error of u is in the order of 10^{-5}.

Example 2

Let us consider the following Carrier-Pearson problem (Carrier and Pearson, 1991):

$$\varepsilon u'' = 1 - u^2, \tag{122}$$

$$u(-1) = 0, \quad u(1) = 0, \tag{123}$$

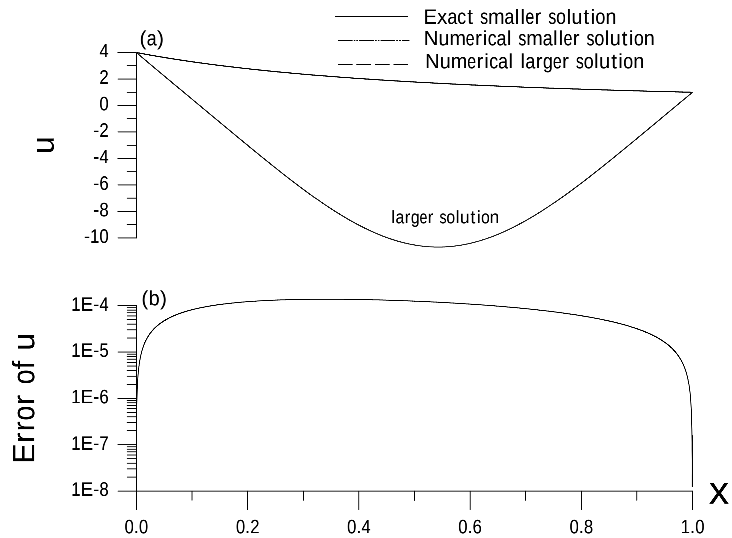

Figure 2: Comparing numerical solutions and exact solutions for Example 1 in (a), and (b) the numerical error.

where ε is a small parameter.

This problem is very complex when ε is small. Here we only show two different solutions in Fig. 3 with $\varepsilon = 0.1$. The solution with positive slope is obtained by taking $r = 0.88111263$ and the one with negative slope is obtained by taking $r = 0.9583918$. In these calculations the translation constant $c = 20$ was used, and the stepsize used was $h = 0.00001$.

Example 3

Let us consider the following BVP (Kubicek and Hlavacek, 1983):

$$u'' + \frac{1}{x}u' = -\delta e^{u}, \tag{124}$$

$$u'(0) = 0, \quad u(1) = 0. \tag{125}$$

This problem is of the first Robin type and is singular at the zero point $x = 0$. This equation is simply transformed by $x = t$ and $y = u + c$ into Eqs. (15) and (16) with

$$f_2(t, y, \dot{y}) = -\delta e^{y-c} - \frac{1}{t}\dot{y}, \quad -1 \le t \le 1. \tag{126}$$

The closed form solution of Eq. (124) is

$$u(x) = \ln \frac{8\rho}{\delta(1+\rho x^2)^2}, \tag{127}$$

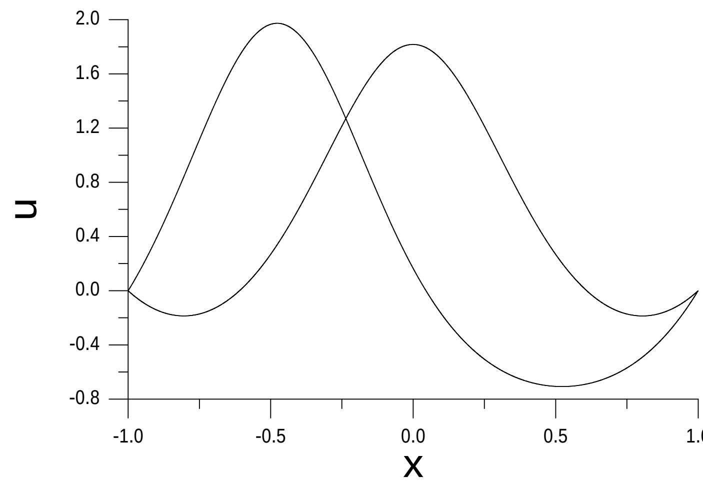

Figure 3: For Example 2 we plot two numerical solutions one with $A > 0$ and another with $A < 0$.

where the integration constant ρ is determined by

$$\frac{8\rho}{\delta(1+\rho)^2} = 1. \tag{128}$$

It can be seen that for a given δ in the range of $0 < \delta < 2$, two distinct real roots of ρ in Eq. (128) exist:

$$\rho_1 = \frac{1}{2}\left[\frac{8}{\delta} - 2 + \sqrt{\left(\frac{8}{\delta} - 2\right)^2 - 4}\right],$$

$$\rho_2 = \frac{1}{2}\left[\frac{8}{\delta} - 2 - \sqrt{\left(\frac{8}{\delta} - 2\right)^2 - 4}\right],$$

and correspondingly, there are two solutions in Eq. (127). For $\delta = 2$, there is only one solution corresponding to $\rho = 1$.

For each given r we use Eq. (99) to calculate A, and then numerically integrate the IVP by the numerical scheme in Section 6.1. For $\delta = 1.8$ we plot the curve of A with respect to r in Fig. 4(a), and the curve of $y_2(0)$ with respect to r in Fig. 4(b). In this calculation we have fixed $c = 1$ and the stepsize $h = 0.0001$. It can be seen that there are two roots of r, of which the target equation $y_2(0) = 0$ is satisfied as shown in Fig. 4(b) by intersecting the curve with the zero line.

Then, we apply the Lie-group shooting technique to this problem for searching the missing initial condition $y_2(-1) = A$. In Fig. 5 we compare our solutions with

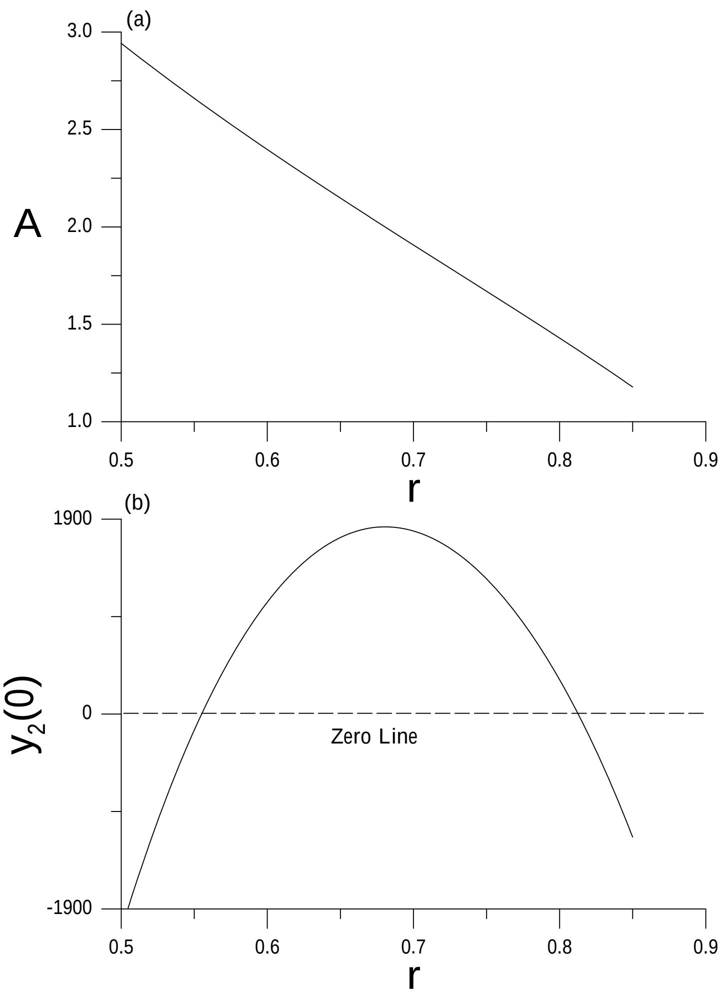

Figure 4: For Example 3 we plot A with respect to r in (a), and $y_2(0)$ with respect to r in (b), where the intersection points locate the roots of r.

the exact solutions by taking $\delta = 1.8$ and $r = 0.8127308556$ for smaller solution and $r = 0.55507615685$ for larger solution. They lead to the errors of the value of $y_2(0)$ in the order of 10^{-7} when compared with the exact $y_2(0) = 0$. It can be seen that the numerical errors of u are both in the order of 10^{-5}. In Fig. 5(a) we also plotted the symmetric solutions of $u = y - c$ in the range of $t \in [-1, 1]$. It can be seen that the curves are perfectly symmetric, and $\dot{u}(0) = 0$ is fulfilled exactly.

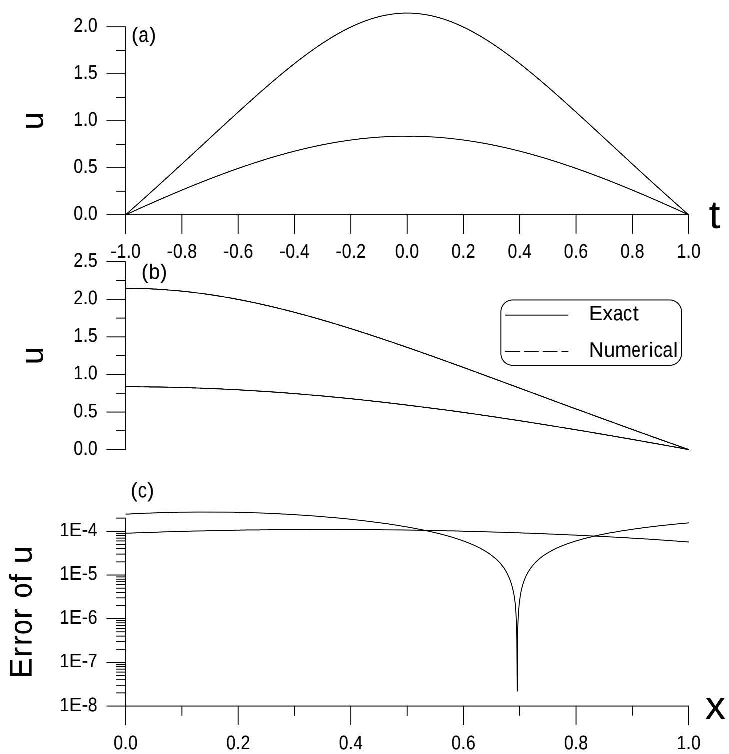

Figure 5: For Example 3: (a) plotting numerical solutions with respect to t, (b) comparing numerical solutions and exact solutions with respect to x, and (c) the numerical errors.

Example 4

Let us consider the following BVP (Kubicek and Hlavacek, 1983):

$$u'' = a_0^2 u \exp\left[\frac{a_1(1-u)}{1+a_2(1-u)}\right], \tag{129}$$

$$u'(0) = 0, \quad u(1) = 1. \tag{130}$$

This problem is of the first Robin type and has three solutions under $a_0 = 0.16$, $a_1 = 14$ and $a_2 = 0.7$. This equation is simply transformed by $x = t$ and $y = u + c - 1$ into Eqs. (15) and (16) with

$$f_2(t, y, \dot{y}) = a_0^2(y + 1 - c)\exp\left[\frac{a_1(c-y)}{1+a_2(c-y)}\right], \tag{131}$$

$$y(-1) = c, \quad y(1) = c. \tag{132}$$

The shooting method is to match $\dot{y}(0) = 0$.

For each given r we use Eq. (110) to calculate A, and then numerically integrate the IVP by the fourth-order Runge-Kutta method. We plot the curve of A with respect to r in Fig. 6(a), and the curve of $y_2(0)$ with respect to r in Fig. 6(b). In this calculation we have fixed $c = 1$ and the stepsize $h = 0.0001$. It can be seen that there are three roots of r, of which the target equation $y_2(0) = 0$ is satisfied as shown in Fig. 6(b) by intersecting the curve with the zero line.

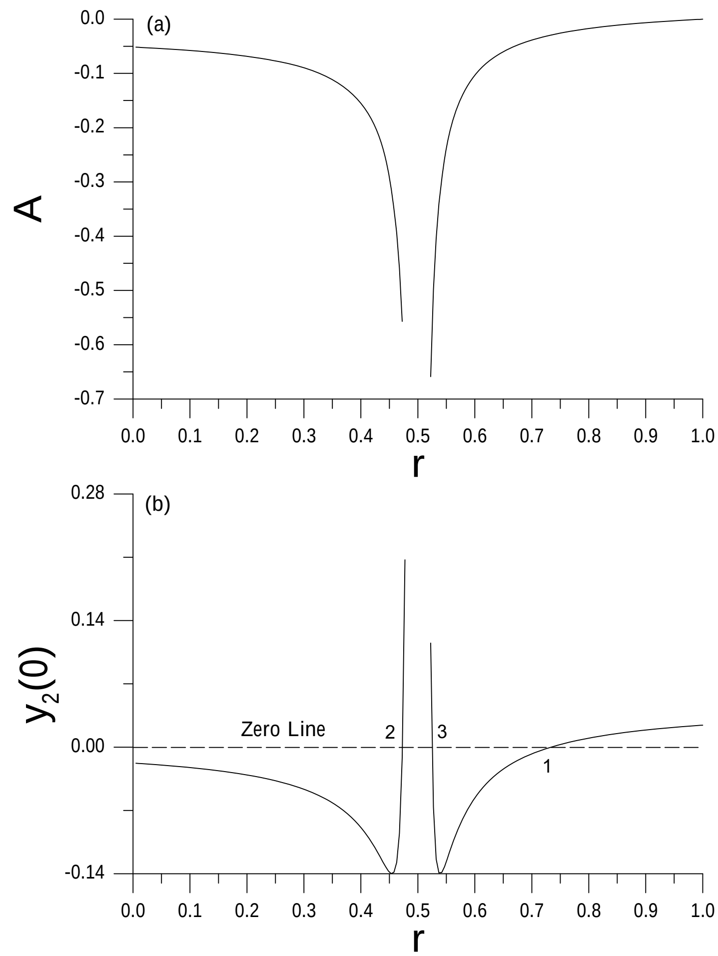

Figure 6: For Example 4 we plot A with respect to r in (a), and $y_2(0)$ with respect to r in (b), where the intersection points locate the roots of r.

We display our solutions by taking $r = 0.7339775983$ at point 1 for the smallest solution as shown in Fig. 7(a), $r = 0.473000077736$ at point 2 for the moderate solution and $r = 0.51386987259$ at point 3 for the largest solution as shown in Fig. 7(b). The largest solution is very sensitive to the disturbance of the slope and we integrate this solution by using $h = 0.00001$.

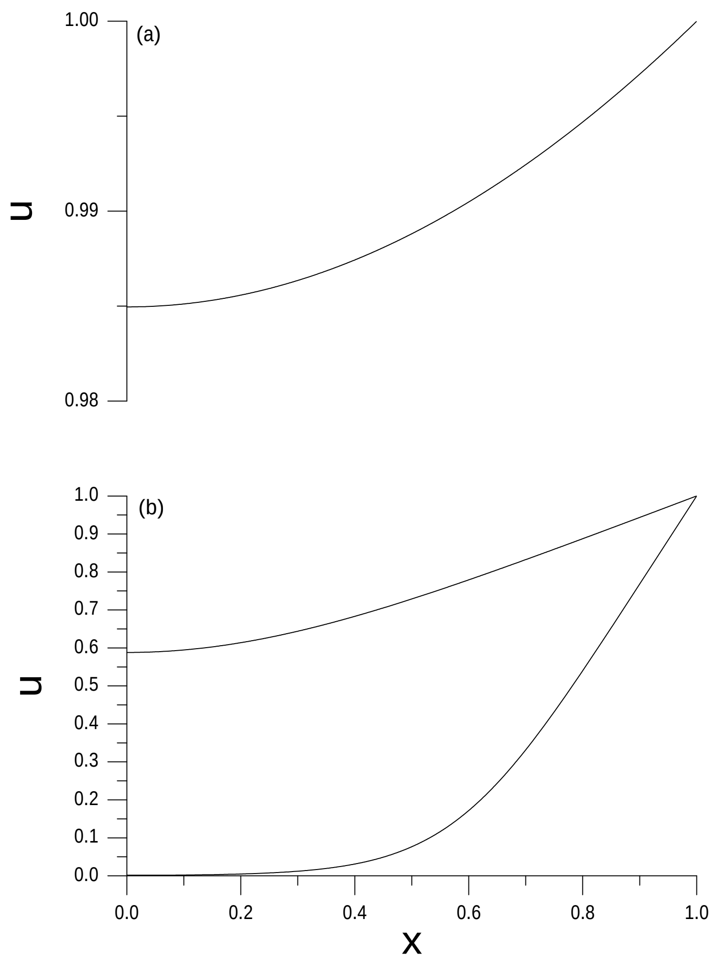

Figure 7: Plotting three numerical solutions for Example 4.

The Neumann problems

The governing equations

In addition Eq. (6) we use the following transformation:

$$y(t) = u(x) + \frac{1}{2}k_1 t^2 + k_2 t = u(x) + \frac{1}{2}(\beta - \alpha)(a-b)t^2 + \alpha(a-b)t, \tag{133}$$

and then, Eqs. (1) and (5) can be reduced to

$$\ddot{y} = f(t, y, \dot{y}), \tag{134}$$

$$\dot{y}(0) = 0, \quad \dot{y}(1) = 0, \tag{135}$$

where

$$f(t,y,\dot{y}) := (b-a)^2 F(a+(b-a)t, y-k_1t^2/2-k_2t, (\dot{y}-k_1t-k_2)/(b-a)+k_1). \tag{136}$$

The equation, required to determine the unknown $y(0)=C$, can be obtained by a similar argument as that in Section 3. For this purpose let us write

$$\dot{y}_1 = y_2, \tag{137}$$

$$\dot{y}_2 = f(t,y_1,y_2), \tag{138}$$

$$y_1(t_0) = C, \quad y_1(1) = D, \tag{139}$$

$$y_2(t_0) = A, \quad y_2(1) = B. \tag{140}$$

In above, $t_0 = 0$ and $A = B = 0$.

From Eq. (62) and

$$\mathbf{y}_0 = \begin{bmatrix} C \\ A \end{bmatrix} = \begin{bmatrix} C \\ 0 \end{bmatrix}, \quad \mathbf{y}_f = \begin{bmatrix} D \\ B \end{bmatrix} = \begin{bmatrix} D \\ 0 \end{bmatrix} \tag{141}$$

it follows that

$$\cos\theta = \frac{C(D-C)+A(B-A)}{\sqrt{(C-D)^2+(A-B)^2}\sqrt{C^2+A^2}}. \tag{142}$$

Because of $A=B=0$, $\cos\theta$ may be -1 or +1. Let us first consider the case of $\cos\theta = -1$, of which $C(D-C)<0$ is deduced. Under this condition from Eq. (66) we obtain

$$Z = \frac{\sqrt{C^2}}{\sqrt{D^2}}. \tag{143}$$

If $C<0$ then $D-C>0$ and from Eqs. (63) and (65) we have

$$S = D-C, \tag{144}$$

$$\eta = \frac{D-C}{\ln\frac{\sqrt{C^2}}{\sqrt{D^2}}}, \tag{145}$$

due to $A=B=0$.

From Eqs. (58), (139), (140) and (51) it follows that

$$\mathbf{F} := \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} = \frac{1}{\eta}\begin{bmatrix} D-C \\ B-A \end{bmatrix} = \frac{1}{\|\hat{\mathbf{y}}\|}\begin{bmatrix} \hat{y}_2 \\ \hat{f} \end{bmatrix}, \tag{146}$$

and that $\hat{y}_1 = rC+(1-r)D$ and $\hat{y}_2 = rA+(1-r)B = 0$, where $\|\hat{\mathbf{y}}\| = \sqrt{\hat{y}_1^2+\hat{y}_2^2} = \sqrt{[rC+(1-r)D]^2} \neq 0$.

From the second equation in Eq. (146) it follows that

$$\hat{f} = f(r, \hat{y}_1, \hat{y}_2) = f(r, rC + (1-r)D, 0) = 0, \tag{147}$$

due to $A = B = 0$.

On the other hand, from the first equation in Eq. (146) we have

$$\frac{1}{\eta}(D-C) = \frac{\hat{y}_2}{\|\hat{\mathbf{y}}\|} = 0, \tag{148}$$

because of $\hat{y}_2 = 0$. Substituting Eq. (145) for η into the above equation we obtain

$$\ln \frac{\sqrt{C^2}}{\sqrt{D^2}} = 0. \tag{149}$$

Therefore, we have $D = -C$, and Eq. (147) can be used to solve C for a given r.

Now, suppose that $C > 0$, and then $D - C < 0$ follows from the inequality $C(D-C) < 0$. Under this condition from Eqs. (66), (63) and (65) we obtain

$$Z = \frac{\sqrt{D^2}}{\sqrt{C^2}}, \tag{150}$$

$$S = C - D, \tag{151}$$

$$\eta = \frac{C-D}{\ln \frac{\sqrt{D^2}}{\sqrt{C^2}}}. \tag{152}$$

A similar argument as that in the above leads to $D = -C$.

The case of $\cos\theta = 1$ implies that $C(D-C) > 0$ by Eq. (142). However, the same argument as that in the above leads to $D = -C$. This results in $C(D-C) = -2C^2 < 0$, which contradicts to $C(D-C) > 0$. It means that there exists no such case that $\cos\theta = 1$.

Therefore, by inserting $D = -C$ into Eq. (147) we have the following equation to solve C:

$$f(r, (2r-1)C, 0) = 0, \tag{153}$$

no matter C is positive or negative. If C is available, we can return to Eqs. (137)-(140) and integrate them by a suitable forward IVP solver with initial conditions $y_1(0) = C$ and $y_2(0) = A = 0$.

Example 5

Let us consider a reaction problem studied by Finlayson (1972). It arises when modeling a tubular reactor with axial dispersion. An isothermal situation with n-th order irreversible reaction leads to

$$u'' = Pe(u' + Ru^n), \tag{154}$$
$$u'(0) = Pe[C-1], \quad u'(1) = 0, \tag{155}$$

where $u(0) = C$ is an unknown constant. In above Pe is the axial Peclet number and R is the reaction rate group.

For this problem we have

$$\alpha = Pe[C-1], \quad \beta = 0.$$

Substituting them into Eq. (133) we obtain

$$y(t) = u(x) + \frac{1}{2}\alpha t^2 - \alpha t. \tag{156}$$

Therefore, we obtain Eqs. (134) and (135) with the following

$$f(t,y,\dot{y}) = \alpha + Pe\left[\dot{y} - \alpha t + \alpha + R\left(y - \frac{1}{2}\alpha t^2 + \alpha t\right)^n\right]. \tag{157}$$

Substituting Eq. (157) into Eq. (153) we obtain

$$f(r,(2r-1)C,0) = \alpha + Pe\left[-r\alpha + \alpha + R\left((2r-1)C - \frac{1}{2}r^2\alpha + r\alpha\right)^n\right] = 0, \tag{158}$$

which for a given r can be used to solve C by inserting $\alpha = Pe[C-1]$.

Then we integrate the following equations:

$$\dot{y}_1 = y_2, \tag{159}$$
$$\dot{y}_2 = \alpha + Pe\left[y_2 - \alpha t + \alpha + R\left(y_1 - \frac{1}{2}\alpha t^2 + \alpha t\right)^n\right], \tag{160}$$
$$y_1(t_0) = C, \tag{161}$$
$$y_2(t_0) = 0, \tag{162}$$

with C given by Eq. (158). Let $r = 0.4180812$ we plot the (x,y) and (x,u) in Fig. 8 under $Pe = 1$, $R = 2$ and $n = 2$. For this case the α can be solved in closed-form:

$$\alpha = \frac{-B_0 - \sqrt{B_0^2 - 4A_0C_0}}{2A_0}, \tag{163}$$
$$A_0 = 2(3r - 1 - 0.5r^2)^2, \tag{164}$$
$$B_0 = 4(2r-1)(3r-1-0.5r^2)^2 + 2 - r, \tag{165}$$
$$C_0 = 2(2r-1)^2. \tag{166}$$

These equations are integrated backward by the numerical method of backward group preserving scheme (BGPS) developed by Liu, Chang and Chang (2006) with the conditions $y(1) = D = -C = -\alpha - 1$ and $y_2(1) = \dot{y}(1) = 0$. It can be seen that the numerical solution exactly satisfies the boundary conditions with $\dot{y}(0) = \dot{y}(1) = 0$ as shown in Fig. 8(a). In our calculation we get $u(0) = 2.798782$ and $u(1) = 1.188085$.

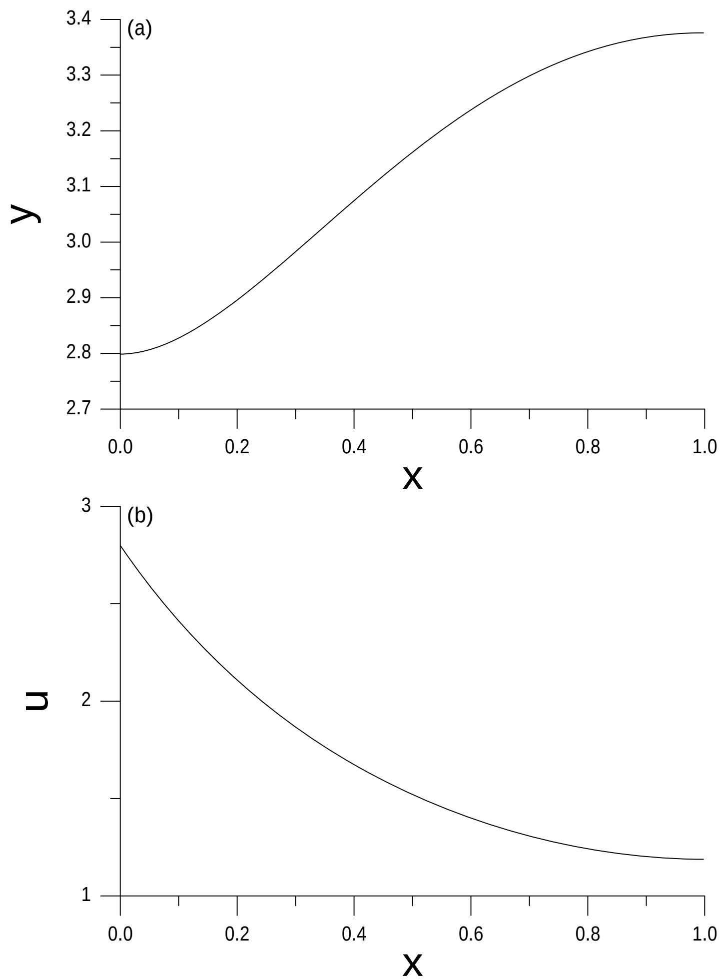

Figure 8: For Example 5: (a) plotting numerical solution of y with respect to x, and (b) plotting numerical solution of u with respect to x.

Conclusions

In this paper we have fully utilized Eqs. (55) and (56) to construct a one-step group element $\mathbf{G}(\mathbf{y}_0, \mathbf{y}_f)$, which is the Lie group transformation between initial point and final point on the cone in the Minkowski space. Then, we used a mean value theorem to construct another Lie group element $\mathbf{G}(r)$. In order to estimate the missing initial conditions for the two-point nonlinear boundary value problems, we have employed the equation $\mathbf{G}(\mathbf{y}_0, \mathbf{y}_f) = \mathbf{G}(r)$ to derive algebraic equations. Through a symmetric extension technique we have transformed the Robin type nonlinear BVPs into a canonical one, which together with the other two type problems all can be solved in closed-form of the unknown initial conditions in terms of r in a compact space of $r \in (0,1)$.

Numerical examples were examined to ensure that the Lie-group shooting method can calculate the solutions of second-order nonlinear BVPs even with multiple solutions. The numerical solutions could match the specified boundary conditions with high accuracy. Through this study, it can be concluded that the Lie-group shooting method is accurate, effective and stable. Its numerical implementation is very simple and the computation speed is very fast to find all possible solutions.

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