# Solving an inverse Sturm-Liouville problem by a Lie-group method

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## Abstract

Solving an inverse Sturm-Liouville problem requires a mathematical process to determine unknown function in the Sturm-Liouville operator from given data in addition the boundary values. In this paper we identify a Sturm-Liouville potential function by using the data of one eigenfunction and its corresponding eigenvalue, and identify a spatial-dependent unknown function of a Sturm-Liouville differential operator. The method we employ is to transform the inverse Sturm-Liouville problem into a parameter identification problem of a heat conduction equation. Then a Lie-group estimation method is developed to estimate the coefficients in a system of ordinary differential equations discretized from that heat conduction equation. Numerical tests confirm the accuracy and efficiency of present approach. Definite and random disturbances are also considered when compare the present method with that by using a technique of numerical differentiation.

## 1 Introduction

The problem to describe the interaction between colliding particles is of fundamental one in the physics of particle, where the identification of Schrödinger operator is utmost important. It is one sort of the inverse Sturm-Liouville problems, which have various versions. Among them the best known one is studied by Gelfand and Levitan [7], in which the potential function is uniquely determined by spectral function. McLaughlin [20] has given an analytical method to treat this type inverse problem.

There were many works to develop algorithms for solving the inverse Sturm-Liouville problem of reconstructing potential function from eigenvalues [2, 22], which is known as the inverse spectral problem or inverse eigenvalue problem [6]. On the other hand, McLaughlin [21] first noted that it is possible to obtain the potential function and boundary conditions using only the set of nodal points. This interesting problem is soon knowing as the inverse nodal problem [4, 5, 8, 24].

Numerical methods often transform the inverse Sturm-Liouville problem into an inverse eigenvalue problem of a certain matrix [3]. However, many of these discretizations into a matrix form have higher eigenvalues significantly differing from those of true eigenvalues. As a consequence, the inverse algorithms based on these discretizations require careful implementation [2, 22].

In this study the data of spectral function is chosen in order to identify a spatial-dependent potential function; hence, the present inverse Sturm-Liouville problem is less

difficult than those considered in [2, 4, 5, 8, 21, 22, 24].

First, we transform the inverse Sturm-Liouville problem into a parameter identification problem governed by a parabolic type partial differential equation (PDE). Then, a one-step group-preserving scheme (GPS) for a semi-discretization of that PDE is established, which can be used to derive a closed-form solution of the estimated potential function at discretized spatial points. This type approach is first time appeared in the literature.

Let us consider a second-order ordinary differential equation (ODE) describing the Sturm-Liouville boundary value problem:

$$\frac{d}{dx}\left[p(x)\frac{dy}{dx}\right] + [q(x) + \lambda r(x)]y = F(x) \quad \text{in} \quad x_0 \leq x \leq x_f, \tag{1}$$

$$y = A_0 \quad \text{at} \quad x = x_0, \tag{2}$$

$$y = B_0 \quad \text{at} \quad x = x_f. \tag{3}$$

The direct problem is for the given conditions in Eqs. (2) and (3) and the given functions $p(x)$, $q(x)$, $r(x)$ and $F(x)$ to find the solution $y(x)$ of the second-order boundary value problem (BVP). Specifically, when $F(x) = 0$ we have a Sturm-Liouville problem to determine the eigenvalue $\lambda$ and eigenfunction $y(x)$.

The present inverse problem of Sturm-Liouville is to estimate $q(x)$ by using the information of one eigenfunction $y(x)$ and its corresponding eigenvalue $\lambda$, and for the Sturm-Liouville differential operator is to estimate $p(x)$ by using the data of $y(x)$ when $q(x) = r(x) = 0$.

For the case when $p(x_f)$ is known and $q(x) = r(x) = 0$ in Eq. (1), we propose a non-iterative method to calculate $p(x)$ at discretized spatial points. This problem could also be solved by the iterative method given by Keung and Zou [11] for the elliptic problem $\nabla \cdot (p\nabla u) = F$. Some of the numerical examples in Keung and Zou [11] involve Sturm-Liouville problems, but the method proposed here requires less computation for these problems.

For the case of $q(x) = r(x) = 0$ from Eq. (1) it follows directly that

$$p(x)y'(x) = p(x_0)y'(x_0) + \int_{x_0}^{x} F(s)ds. \tag{4}$$

If $y'(x)$, $p(x_0)$ and $y'(x_0)$ are available, the above equation simply gives the unknown parameter $p(x)$ by dividing both the sides by $y'(x)$. However, because $y(x)$ is usually not given in a closed-form and is given discretizedly under a perturbation by noise, we require a numerical technique to find $y'(x)$. As mentioned by Li [12] several techniques were developed to construct useful difference formulas for numerical derivatives (ND). In addition to the references in [12], we also mention the book by Shu [23]. Among the many NDs we only employ the method by Ahn et al. [1] to compare it with our new method for numerical examples given in Section 6. Ahn et al. [1] have used a Volterra integral equation of the second kind to derive the following numerical derivative of a function $f(x)$ under noise denoted by $f_\delta(x)$:

$$f'_\delta(x) = \frac{-1}{\alpha^2}\exp\left(\frac{-x}{\alpha}\right)\int_0^x \exp\left(\frac{s}{\alpha}\right)f_\delta(s)ds + \frac{f_\delta(x)}{\alpha}, \tag{5}$$

where $\alpha$ is a regularized parameter, and $f'_\delta(x)$ is a numerical derivative of $f_\delta(x)$.

Lie-group is a differentiable manifold, endowed a group structure that is compatible with the underlying topology of manifold. The main purpose of Lie-group solver is for providing a better algorithm that retains the orbit generated from numerical solution on the manifold which associated with the Lie-group [9, 17]. The retention of Lie-group structure under

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discretization is vital in the recovery of qualitatively correct behavior in the minimization of numerical error [10, 13].

Liu [14] has extended the GPS developed in [13] for ODEs to solve the BVPs, and the numerical results reveal that the GPS is a rather promising method to effectively solve the two-point BVPs. In that construction of Lie-group method for the calculations of BVPs, Liu [14] 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.

It should be stressed that the one-step property of Lie-group is usually not shared by other numerical methods, because those methods do not belong to the Lie-group type. This important property has been used by Liu [15] to establish a one-step estimation method to estimate the temperature-dependent heat conductivity, and then extended to estimate heat conductivity and heat capacity [16, 18, 19]. Its group structure gives the Lie-group method a great advantage over other numerical methods. It is a powerful technique to solve the inverse problem of parameter identification.

This paper is arranged as follows. We introduce a novel approach of an inverse Sturm-Liouville problem in Section 2 by transforming it into an identification problem of a parabolic type PDE, and then discretizing the PDE into a system of ODEs at discretized spatial points. In Section 3 we give a brief sketch of the GPS for ODEs for a self-content reason. Due to its good property of Lie-group, we will propose a one-step GPS, which can be used to identify the parameters appeared in the PDE. The resulting algebraic equation is derived in Section 4 when we apply the one-step GPS to identify $q(x)$. We demonstrate that how the Lie-group theory can help us to solve the parameter estimation equation in a closed-form. In Section 5 we turn our attention to the estimation of $p(x)$, which leads again to a closed-form solution of the parameter $p(x)$ at discretized spatial points. In Section 6 several numerical examples are examined to test the Lie-group estimation method (LGEM). Finally, we give conclusions in Section 7.

## 2 A novel approach

### 2.1. Transformation into a PDE

In the solution of linear PDE, a common technique is the seperation of variables, from which the PDE is transformed into ODEs. We may reverse this process by considering

$$u(x,t) = (1+t)y(x), \tag{6}$$

such that Eqs. (1)-(3) are changed to

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[p(x)\frac{\partial u(x,t)}{\partial x}\right] + [q(x) + \lambda r(x)]u(x,t) + h(x,t)$$

$$\text{in} \ \ x_0 \le x \le x_f, \ \ 0 < t \le T, \tag{7}$$

$$u(x_0, t) = A_0(1+t), \tag{8}$$

$$u(x_f, t) = B_0(1+t), \tag{9}$$

$$u(x, 0) = y(x), \tag{10}$$

where $h(x,t) = y(x) - (1+t)F(x)$, and the last initial condition follows from Eq. (6) directly.

Eq. (7) is a heat conduction equation, where we are attempting to estimate $p(x)$ or $q(x)$ under a given source $h(x,t)$.

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## 2.2. Semi-Discretization

The semi-discrete procedure of PDE produces a coupled system of ODEs. For the one-dimensional heat conduction equation (7), we adopt the numerical method of line to discretize the spatial coordinate $x$ by

$$\frac{\partial u(x,t)}{\partial x}\bigg|_{x=x_i=x_0+i\Delta x} = \frac{u_{i+1}(t) - u_i(t)}{\Delta x}, \tag{11}$$

$$\frac{\partial^2 u(x,t)}{\partial x^2}\bigg|_{x=x_i=x_0+i\Delta x} = \frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{(\Delta x)^2}, \tag{12}$$

where $\Delta x = (x_f - x_0)/(n + 1)$ is a uniform discretization spacing length, and $u_i(t) = u(x_0 + i\Delta x, t)$ for a simple notation. Such that Eq. (7) can be approximated by

$$\begin{aligned}
\dot{u}_i(t) &= \frac{p_i}{(\Delta x)^2}[u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)] \\
&+ p_i'\frac{u_{i+1}(t) - u_i(t)}{\Delta x} + (q_i + \lambda r_i)u_i(t) + h_i(t), \quad i = 1, \ldots, n,
\end{aligned} \tag{13}$$

where $p_i = p(x_i)$, $p_i' = p'(x_i)$, $q_i = q(x_i)$, $r_i = r(x_i)$, and $h_i(t) = y_i - (1+t)F_i$ with $y_i = y(x_i)$ and $F_i = F(x_i)$.

When $i = 1$ the term $u_0(t)$ is determined by boundary condition (8) with $u_0(t) = A_0(1 + t)$. Similarly, when $i = n$ the term $u_{n+1}(t)$ is determined by boundary condition (9) with $u_{n+1}(t) = B_0(1 + t)$. The next step is to advance the solution from a given initial condition to a desired time $T$. Eq. (13) has totally $n$ coupled linear ODEs for the $n$ variables $u_i(t), i = 1, \ldots, n$, which can be numerically integrated to obtain $u_i(T)$.

In this section we have transformed the inverse Sturm-Liouville problem in Eq. (1) into an inverse parameter identified problem for the PDE in Eq. (7), and finally to an estimation of $n$ coefficients $q_i$ or $p_i$ in the $n$-dimensional linear ODEs system. The data required in the estimation are the discretization of $y(x)$ at discretized spatial points, i.e., $y_i = y(x_i)$.

## 3 GPS for differential equations system

### 3.1. Group-preserving scheme

Upon letting $\mathbf{u} = (u_1, \ldots, u_n)^{\mathrm{T}}$ and denoting $\mathbf{f}$ the right-hand side of Eq. (13) we can write it as a vector form:

$$\dot{\mathbf{u}} = \mathbf{f}(\mathbf{u}, t), \quad \mathbf{u} \in \mathbb{R}^n, \quad t \in \mathbb{R}. \tag{14}$$

Liu [13] has embedded Eq. (14) into an augmented dynamical system, which is concerned with not only the evolution of state variables but also the evolution of the magnitude of the state variables vector:

$$\frac{d}{dt}\begin{bmatrix} \mathbf{u} \\ \|\mathbf{u}\| \end{bmatrix} = \begin{bmatrix} \mathbf{0}_{n\times n} & \frac{\mathbf{f}(\mathbf{u},t)}{\|\mathbf{u}\|} \\ \frac{\mathbf{f}^{\mathrm{T}}(\mathbf{u},t)}{\|\mathbf{u}\|} & 0 \end{bmatrix}\begin{bmatrix} \mathbf{u} \\ \|\mathbf{u}\| \end{bmatrix}. \tag{15}$$

Eq. (15) gives us a Minkowskian structure of the augmented state variables of $\mathbf{X} := (\mathbf{u}^{\mathrm{T}}, \|\mathbf{u}\|)^{\mathrm{T}}$ to satisfy the cone condition:

$$\mathbf{X}^{\mathrm{T}}\mathbf{g}\mathbf{X} = 0, \tag{16}$$

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where

$$\mathbf{g} = \begin{bmatrix} \mathbf{I}_n & \mathbf{0}_{n \times 1} \\ \mathbf{0}_{1 \times n} & -1 \end{bmatrix} \tag{17}$$

is a Minkowski metric, $\mathbf{I}_n$ is the identity matrix of order $n$, and the superscript T stands for the transpose. In terms of $(\mathbf{u}, \|\mathbf{u}\|)$, Eq. (16) becomes

$$\mathbf{X}^{\mathrm{T}}\mathbf{g}\mathbf{X} = \mathbf{u} \cdot \mathbf{u} - \|\mathbf{u}\|^2 = \|\mathbf{u}\|^2 - \|\mathbf{u}\|^2 = 0, \tag{18}$$

where the dot between two $n$-dimensional vectors denotes their Euclidean inner product. The cone condition is thus the most natural constraint that we can impose on the dynamical system (15).

Consequently, we have an $n + 1$-dimensional augmented system:

$$\dot{\mathbf{X}} = \mathbf{A}\mathbf{X} \tag{19}$$

with a constraint (16), where

$$\mathbf{A} := \begin{bmatrix} \mathbf{0}_{n \times n} & \frac{\mathbf{f}(\mathbf{u},t)}{\|\mathbf{u}\|} \\ \frac{\mathbf{f}^{\mathrm{T}}(\mathbf{u},t)}{\|\mathbf{u}\|} & 0 \end{bmatrix}, \tag{20}$$

satisfying

$$\mathbf{A}^{\mathrm{T}}\mathbf{g} + \mathbf{g}\mathbf{A} = \mathbf{0}, \tag{21}$$

is a Lie algebra $so(n,1)$ of the proper orthochronous Lorentz group $SO_o(n,1)$.

Although the dimension of the new system is raised one more, it has been shown that the new system has an advantage to permit the group-preserving scheme (GPS) given as follows [13]:

$$\mathbf{X}_{\ell+1} = \mathbf{G}(\ell)\mathbf{X}_\ell, \tag{22}$$
$$\mathbf{G}^{\mathrm{T}}\mathbf{g}\mathbf{G} = \mathbf{g}, \tag{23}$$
$$\det \mathbf{G} = 1, \tag{24}$$
$$G_0^0 > 0, \tag{25}$$

where $G_0^0$ is the 00th component of $\mathbf{G}$, $\mathbf{X}_\ell$ denotes the numerical value of $\mathbf{X}$ at the discrete time $t_\ell$, and $\mathbf{G}(\ell) \in SO_o(n,1)$ is the group value of $\mathbf{G}$ at a time $t_\ell$. If $\mathbf{G}(\ell)$ satisfies the properties in Eqs. (23)-(25), then $\mathbf{X}_\ell$ satisfies the cone condition in Eq. (16).

The Lie-group $\mathbf{G}$ can be generated from $\mathbf{A} \in so(n,1)$ by an exponential mapping,

$$\mathbf{G}(\ell) = \exp[\Delta t \mathbf{A}(\ell)] = \begin{bmatrix} \mathbf{I}_n + \frac{(a_\ell-1)}{\|\mathbf{f}_\ell\|^2}\mathbf{f}_\ell\mathbf{f}_\ell^{\mathrm{T}} & \frac{b_\ell \mathbf{f}_\ell}{\|\mathbf{f}_\ell\|} \\ \frac{b_\ell \mathbf{f}_\ell^{\mathrm{T}}}{\|\mathbf{f}_\ell\|} & a_\ell \end{bmatrix}, \tag{26}$$

where

$$a_\ell := \cosh\left(\frac{\Delta t \|\mathbf{f}_\ell\|}{\|\mathbf{u}_\ell\|}\right), \tag{27}$$

$$b_\ell := \sinh\left(\frac{\Delta t \|\mathbf{f}_\ell\|}{\|\mathbf{u}_\ell\|}\right). \tag{28}$$

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Substituting Eq. (26) for $\mathbf{G}(\ell)$ into Eq. (22), we obtain

$$\mathbf{u}_{\ell+1} = \mathbf{u}_\ell + \eta_\ell \mathbf{f}_\ell, \tag{29}$$

$$\|\mathbf{u}_{\ell+1}\| = a_\ell \|\mathbf{u}_\ell\| + \frac{b_\ell}{\|\mathbf{f}_\ell\|} \mathbf{f}_\ell \cdot \mathbf{u}_\ell, \tag{30}$$

where

$$\eta_\ell := \frac{b_\ell \|\mathbf{u}_\ell\| \|\mathbf{f}_\ell\| + (a_\ell - 1)\mathbf{f}_\ell \cdot \mathbf{u}_\ell}{\|\mathbf{f}_\ell\|^2} \tag{31}$$

is an adaptive factor. From $\mathbf{f}_\ell \cdot \mathbf{u}_\ell \geq -\|\mathbf{f}_\ell\|\|\mathbf{u}_\ell\|$ we can prove that

$$\eta_\ell \geq \left[1 - \exp\left(-\frac{\Delta t \|\mathbf{f}_\ell\|}{\|\mathbf{u}_\ell\|}\right)\right] \frac{\|\mathbf{u}_\ell\|}{\|\mathbf{f}_\ell\|} > 0, \quad \forall \Delta t > 0. \tag{32}$$

This scheme is group properties preserved for all $\Delta t > 0$.

*3.2. One-step GPS*

Applying scheme (29) on Eq. (13) we can compute the heat conduction equation by the GPS. Assume that the total time $T$ is divided by $K$ steps, that is, the time stepsize we use in the GPS is $\Delta t = T/K$.

Starting from an initial augmented condition $\mathbf{X}_0 = \mathbf{X}(0)$ we may want to calculate the value $\mathbf{X}(T)$ at a desired time $t = T$. By Eq. (22) we can obtain

$$\mathbf{X}_T = \mathbf{G}_K(\Delta t) \cdots \mathbf{G}_1(\Delta t)\mathbf{X}_0, \tag{33}$$

where $\mathbf{X}_T$ approximates the real $\mathbf{X}(T)$ within a certain accuracy depending on $\Delta t$. However, let us recall that each $\mathbf{G}_i$, $i = 1, \ldots, K$, is an element of the Lie-group $SO_o(n, 1)$, 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 $\mathbf{G}(T)$. Hence, we have

$$\mathbf{X}_T = \mathbf{G}(T)\mathbf{X}_0. \tag{34}$$

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

Usually, it is very hard to find an exact solution of $\mathbf{G}(T)$; however, a numerical one may be obtained approximately without any difficulty. The most simple method to calculate $\mathbf{G}(T)$ is given by

$$\mathbf{G}(T) = \begin{bmatrix} \mathbf{I}_n + \frac{(a-1)}{\|\mathbf{f}_0\|^2}\mathbf{f}_0\mathbf{f}_0^{\mathrm{T}} & \frac{b\mathbf{f}_0}{\|\mathbf{f}_0\|} \\ \frac{b\mathbf{f}_0^{\mathrm{T}}}{\|\mathbf{f}_0\|} & a \end{bmatrix}, \tag{35}$$

where

$$a := \cosh\left(\frac{T\|\mathbf{f}_0\|}{\|\mathbf{u}_0\|}\right), \tag{36}$$

$$b := \sinh\left(\frac{T\|\mathbf{f}_0\|}{\|\mathbf{u}_0\|}\right). \tag{37}$$

Then from Eqs. (29) and (30) we obtain a one-step GPS:

$$\mathbf{u}_T = \mathbf{u}_0 + \eta \mathbf{f}_0, \tag{38}$$

$$\|\mathbf{u}_T\| = a\|\mathbf{u}_0\| + \frac{b\mathbf{f}_0 \cdot \mathbf{u}_0}{\|\mathbf{f}_0\|}, \tag{39}$$

where

$$\eta = \frac{(a-1)\mathbf{f}_0 \cdot \mathbf{u}_0 + b\|\mathbf{u}_0\|\|\mathbf{f}_0\|}{\|\mathbf{f}_0\|^2}. \tag{40}$$

## 4 Identifying $q(x)$ by the LGEM

In this section we will start to estimate the potential function $q(x)$. By using the one-step GPS we also suppose that the initial value of $u(x, 0) = y(x)$ is given and its corresponding eigenvalue is known.

Applying the one-step GPS in Eq. (38) on Eq. (13) from time $t = 0$ to time $t = T$ we obtain a nonlinear equation for $q_i$:

$$u_i^T = u_i^0 + \frac{\eta p_i}{(\Delta x)^2}(u_{i+1}^0 - 2u_i^0 + u_{i-1}^0) + \eta p_i' \frac{u_{i+1}^0 - u_i^0}{\Delta x} + \eta(q_i + \lambda r_i)u_i^0 + \eta h_i(0). \tag{41}$$

It is not difficult to rewrite Eq. (41) as

$$q_i = \frac{1}{u_i^0}\left[\frac{u_i^T - u_i^0}{\eta} - \frac{p_i}{(\Delta x)^2}(u_{i+1}^0 - 2u_i^0 + u_{i-1}^0) - \frac{p_i'}{\Delta x}(u_{i+1}^0 - u_i^0) - \lambda r_i u_i^0 - h_i(0)\right]. \tag{42}$$

$\eta$ in the above is not a constant but a nonlinear function of $q_i$ as shown by Eq. (40). Therefore in this stage we cannot calculate $q_i$ by a simple equation. However, we will prove below that $\eta$ is fully determined by $u_i^0$ and $u_i^T$.

In order to solve $q_i$, let us return to Eq. (38):

$$\mathbf{f}_0 = \frac{1}{\eta}[\mathbf{u}_T - \mathbf{u}_0]. \tag{43}$$

Substituting it for $\mathbf{f}_0$ into Eq. (39) we obtain

$$\frac{\|\mathbf{u}_T\|}{\|\mathbf{u}_0\|} = a + \frac{b[\mathbf{u}_T - \mathbf{u}_0] \cdot \mathbf{u}_0}{\|\mathbf{u}_T - \mathbf{u}_0\|\|\mathbf{u}_0\|}, \tag{44}$$

where

$$a := \cosh\left(\frac{T\|\mathbf{u}_T - \mathbf{u}_0\|}{\eta\|\mathbf{u}_0\|}\right), \tag{45}$$

$$b := \sinh\left(\frac{T\|\mathbf{u}_T - \mathbf{u}_0\|}{\eta\|\mathbf{u}_0\|}\right). \tag{46}$$

Let

$$\cos\theta := \frac{[\mathbf{u}_T - \mathbf{u}_0] \cdot \mathbf{u}_0}{\|\mathbf{u}_T - \mathbf{u}_0\|\|\mathbf{u}_0\|}, \tag{47}$$

$$S := \frac{T\|\mathbf{u}_T - \mathbf{u}_0\|}{\|\mathbf{u}_0\|}, \tag{48}$$

and from Eqs. (44)-(46) it follows that

$$\frac{\|\mathbf{u}_T\|}{\|\mathbf{u}_0\|} = \cosh\left(\frac{S}{\eta}\right) + \cos\theta \sinh\left(\frac{S}{\eta}\right). \tag{49}$$

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Upon defining

$$Z := \exp\left(\frac{S}{\eta}\right), \tag{50}$$

from Eq. (49) we obtain a quadratic equation for $Z$:

$$(1 + \cos\theta)Z^2 - \frac{2\|\mathbf{u}_T\|}{\|\mathbf{u}_0\|}Z + 1 - \cos\theta = 0. \tag{51}$$

The solution is found to be

$$Z = \frac{\frac{\|\mathbf{u}_T\|}{\|\mathbf{u}_0\|} \pm \sqrt{\left(\frac{\|\mathbf{u}_T\|}{\|\mathbf{u}_0\|}\right)^2 - (1 - \cos^2\theta)}}{1 + \cos\theta}, \quad \text{if} \quad \pm\cos\theta > 0, \tag{52}$$

and from Eq. (50) we obtain a closed-form solution of $\eta$:

$$\eta = \frac{T\|\mathbf{u}_T - \mathbf{u}_0\|}{\|\mathbf{u}_0\| \ln Z}. \tag{53}$$

Up to here we must point out that for a given $T$, $\eta$ is fully determined by $\mathbf{u}_0$ and $\mathbf{u}_T$, which are supposed to be known. Therefore, the original nonlinear equation (42) becomes a linear equation for $q_i$.

By using Eq. (6) we have

$$u_i^T = (1 + T)u_i^0 = (1 + T)y_i, \tag{54}$$

and thus the vector $\mathbf{u}_T$ is proportional to $\mathbf{u}_0$ with a multiplier $1 + T$ larger than 1. Under this condition we have $\cos\theta = 1$ and $Z$ is given by

$$Z = \frac{\|\mathbf{u}_T\|}{\|\mathbf{u}_0\|} = 1 + T, \tag{55}$$

and hence from Eq. (53) we have

$$\eta = \frac{T^2}{\ln(1 + T)}. \tag{56}$$

Inserting Eqs. (54) and (56) into Eq. (42) we obtain a very simple formula to estimate $q_i$ by

$$q_i = \frac{1}{y_i}\left[\frac{y_i \ln(1 + T)}{T} - \frac{p_i}{(\Delta x)^2}(y_{i+1} - 2y_i + y_{i-1}) - \frac{p_i'}{\Delta x}(y_{i+1} - y_i) - \lambda r_i y_i - y_i + F_i\right]. \tag{57}$$

This solution is in a closed-form for $q_i$.

In the above we have mentioned that $\eta$ is a nonlinear function of $q_i$; however, by viewing Eqs. (47), (52) and (53) it is known that $\eta$ is fully determined by $\mathbf{u}_0$ and $\mathbf{u}_T$. Furthermore, by using Eq. (54) $\eta$ becomes a constant given by Eq. (56). This point is very important for our closed-form solution of parameter. The key points rely on the construction of the method by using the one-step GPS for the estimation of parameter, and the full use of the $n + 1$ equations (38) and (39). To distinguish the present method by a joint use of the one-step GPS and the closed-form solution with the aid of Eq. (39), we may call the new method a Lie-group estimation method (LGEM).

## 5 Applying the LGEM to estimate $p(x)$

In this section we will derive a simple linear equations system to solve the coefficients $p_i$, $i = 1, \ldots, n$. However, for simplicity we assume $q(x) = r(x) = 0$ in this section.

A similar finite difference as that used in Eq. (11) for $u'(x)$ can be used for $p'(x)$ in Eq. (13). In doing so, we can obtain a system of ODEs for $u$ with $t$ as an independent variable:

$$\dot{u}_i(t) = \frac{p_{i+1} - p_i}{\Delta x} \frac{u_{i+1}(t) - u_i(t)}{\Delta x} + p_i \frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{(\Delta x)^2} + h_i(t). \tag{58}$$

The known initial condition is given by

$$u_i^0 = y(x_i), \quad i = 1, \ldots, n, \tag{59}$$

which is obtained from Eq. (6) by a discretization.

Applying the same idea of LGEM on Eq. (58) we can obtain a closed-form formula to estimate $p_i$:

$$p_i = \frac{(\Delta x)^2}{u_i^0 - u_{i-1}^0} \left[ \frac{u_{i+1}^0 - u_i^0}{(\Delta x)^2} p_{i+1} + h_i(0) - \frac{1}{\eta}(u_i^T - u_i^0) \right], \tag{60}$$

and moreover, by using the data of $u_i^T$ given by Eq. (54) and Eq. (56) for $\eta$, we can derive a much simple equation for $p_i$:

$$p_i = \frac{(\Delta x)^2}{y_i - y_{i-1}} \left[ \frac{y_{i+1} - y_i}{(\Delta x)^2} p_{i+1} + y_i - F_i - \frac{y_i \ln(1 + T)}{T} \right]. \tag{61}$$

This will be called a closed-form estimation method. The above equation can be used sequentially to find $p_i$, $i = n, \ldots, 1$ if we know $p_{n+1}$ a priori. Here, $p_{n+1}$ is the right-end boundary value of $p(x)$, and is supposed to be known for simplicity.

However, we can develop another estimation method through iterations. The numerical procedures for estimating $p_i$ are described as follows. We assume an initial value of $p_i$, for example, $p_i = 1$. Substituting it into Eq. (58) we can apply the GPS to integrate it from $t = 0$ to $t = T$ through $T/\Delta t$ steps. Then, we obtain $u_i^T$. Inserting it into Eq. (60) we can calculate a new $p_i$, which is then compared with the old $p_i$. If the difference of these two sets of $p_i$ is smaller than a given criterion, then we stop the iteration and the final $p_i$ is obtained.

The processes are summarized as follows:

(i) Give an initial $p_i = 1$.

(ii) For $j = 1, 2 \ldots$ we repeat the following calculations. Calculate $u_i^T$ by using the GPS in Eq. (29) to integrate Eq. (58) from $t = 0$ to $t = T$, where $\mathbf{f}$ is a vector form of the right-hand side of Eq. (58).

(iii) Insert the above calculated $u_i^T$ denoted by $u_i^T(j)$ together with $u_i^0$ given by Eq. (59) into

$$p_i^j = \frac{(\Delta x)^2}{u_i^0 - u_{i-1}^0} \left[ \frac{u_{i+1}^0 - u_i^0}{(\Delta x)^2} p_{i+1}^j - \frac{1}{\eta^j}[u_i^T(j) - u_i^0] + h_i(0) \right], \tag{62}$$

where $\eta^j$ is calculated from Eq. (53) by substituting $\mathbf{u}_T^j$ for each step. If $p_i^j$ converges according to a given stopping criterion:

$$\sum_{i=1}^{n} (p_i^{j+1} - p_i^j)^2 < \varepsilon^2, \tag{63}$$

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then stop; otherwise, go to step (ii).

Basically, the present method is repeatedly used the time direction integration of Eq. (58) to obtain the final time data to adjust $p_i$, which will be called an iterative estimation method.

## 6 Numerical examples

*6.1. Example 1*

For a first example we consider an inverse Sturm-Liouville problem to identify the potential function in the Schrödinger equation

$$y''(x) + (\beta - \alpha^2 x^2)y(x) = 0, \tag{64}$$
$$y(-\infty) = y(\infty) = 0. \tag{65}$$

Here $\beta = (2k + 1)\alpha$ is the eigenvalue, and

$$y_k(x) = H_k(x) \exp\left(-\frac{\alpha x^2}{2}\right) \tag{66}$$

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

$$H_0(x) = 1, \tag{67}$$
$$H_1(x) = 2x, \tag{68}$$
$$H_2(x) = -2 + 4x^2, \tag{69}$$
$$H_3(x) = -12x + 8x^3, \tag{70}$$
$$H_4(x) = 12 - 48x^2 + 16x^4. \tag{71}$$

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

In order to recover the potential function $q(x)$ from the given eigenvalue and eigenfunction we apply Eq. (57) on this problem by taking $p = 1$, $p' = 0$, $r = 1$ and $F = 0$. We also take $x_0 = -5$ and $x_f = 5$ and let $\Delta x = 10/300$, $\alpha = 1$ and $T = 0.0001$.

The estimation errors of $q(x)$ are shown in Figs. 1(a) and 1(b), for $k = 1$ and $y_1(x)$ and $k = 3$ and $y_3(x)$ as the inputs on Eq. (57). From these two figures it can be seen that the estimations of $q(x)$ are quite accurate. However, near the boundaries the errors are increased. In order to avoid the boundary effect on the estimation of $q(x)$ we can extend the range of $x$ into a larger one.

*6.2 Example 2*

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

$$[x^{-1}y'(x)]' + (\lambda + 1)x^{-3}y(x) = 0, \tag{72}$$
$$y(1) = y(e) = 0. \tag{73}$$

The eigenvalue is $\lambda_k = k^2\pi^2$, $k \in \mathbb{N}$, and the eigenfunction is $y_k = ax\sin(k\pi \ln x)$, where $a$ is an arbitrary nonzero constant fixed to be $a = 100$.

In Fig. 2 we compare the estimation errors by considering the noisy data with $y_\sigma = ax\sin(\pi \ln x) + \sigma R(i)$, where $R(i)$ are random number between -1 and +1. The $L^2$ errors for

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$\sigma = 0$ is about 0.327 while that for $\sigma = 0.01$ is about 0.373.

### 6.3. Example 3

In this example we estimate $p(x)$ by setting $q(x) = 0$ and $r(x) = 0$. Let us use the following example to demonstrate the process in Section 5. This example is given by

$$p(x) = (x-3)^2, \tag{74}$$

$$F(x) = 6(x-3)^2, \quad h(x,t) = y(x) - (1+t)F(x) = -(x-3)^2(5+6t). \tag{75}$$

Under the boundary conditions

$$u(0,t) = 9(1+t), \quad u(1,t) = 4(1+t), \tag{76}$$

and the initial condition

$$u(x,0) = (x-3)^2, \tag{77}$$

the exact solution is given by

$$u(x,t) = (x-3)^2(1+t). \tag{78}$$

We apply the LGEM on this identification of $p(x)$, where we have fixed $\Delta x = 1/30$, $\Delta t = 5 \times 10^{-5}$ and $T = 0.01$. Under the stopping criterion with $\epsilon = 10^{-3}$, the process is convergent within 34 iterations. In Fig. 3(a) we plot the tentative $p_i$ for the first iteration, the fifth iteration, the tenth iteration and the fifteenth iteration, the last of which is already close to the exact solution. The numerical solutions of $p_i$ are close to the exact ones with the $L^2$-norm error about 0.0156, and the maximum relative error about $4 \times 10^{-3}$ as shown in Fig. 3(b).

### 6.4. Example 4

The following example has been calculated by Keung and Zou [11] using the augmented Lagrange method:

$$p(x) = 3 + 2x^2 - 2\sin(2\pi x), \tag{79}$$

$$F(x) = 2\pi[4x - 4\pi\cos(2\pi x)]\cos(2\pi x) - 4\pi^2[3 + 2x^2 - 2\sin(2\pi x)]\sin(2\pi x). \tag{80}$$

The exact solution is given by

$$u(x,t) = (1+t)\sin(2\pi x). \tag{81}$$

We first apply the iterative LGEM on this identification of $p(x)$, where we have fixed $\Delta x = 2/60$, $\Delta t = 10^{-5}$ and $T = 0.003$. Under the stopping criterion with $\epsilon = 10^{-3}$, the process is convergent within 37 iterations. In Fig. 4 we compare the estimated solution with exact solution. For this estimation we have a maximum error with 0.377 and an $L^2$ error with 1.62. On the other hand we also apply Eq. (61) on this estimation by using $\Delta x = 2.2/150$ and $T = 0.001$, of which the result is shown in Fig. 4 by the dashed-dotted line. For the later estimation we have a maximum error with 0.59 and an $L^2$ error with 1.402. It is slightly accurate than the iterative method; however, there appear four kinks near the extremal points

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of $p(x)$, where $p'(x) = 0$.

*6.5. Example 5*

For this example we consider a simple exact $y(x) = \sin(\pi x)$ under a noise given by $y_\delta = \sin(\pi x) + \delta \cos(3\pi x)$. The following results are used:

$$p(x) = x, \tag{82}$$

$$F(x) = \pi \cos(\pi x) - \pi^2 x \sin(\pi x). \tag{83}$$

For the integration in Eq. (5), we have employed the trapezoidal rule to calculate $y_\delta'(x)$ at discretized spatial points. Then inserting them into Eq. (4) we can obtain $p(x)$ by the ND method under $\delta = 0$ and $\delta = 0.02$, whose errors are shown in Fig. 5(a). The best parameter $\alpha$ is fixed to be 0.95 for $\delta = 0$ and 0.85 for $\delta = 0.02$, not 0.0085 as that used by Ahn et al. [1].

On the other hand we also apply Eq. (61) on this estimation of $p(x)$ by using $\Delta x = 0.01$ and $T = 0.01$, of which the errors under $\delta = 0$ and $\delta = 0.02$ are shown in Fig. 5(a). It can be seen that the maximum errors of LGEM are much smaller than that obtained by the ND method. Especially, when $\delta = 0$ the LGEM with all its absolute error is smaller than that by the ND method.

For both methods applied in this example we also consider the random noise disturbance given by $y_\sigma = \sin(\pi x_i) + \sigma R(i)$, where $R(i)$ are random number between -1 and +1. In Fig. 5(b) we compare the numerical errors by applying the LGEM and ND for this case under a noise with $\sigma = 0.001$. For the ND the best parameter of $\alpha$ is $\alpha = 0.5$. Obviously, the absolute error of LGEM is smaller than that given by the ND method. This also shows that the method of LGEM can be against the random and also definite disturbances.

*6.6 Example 6*

Let us consider the following linear BVP:

$$xy''(x) + y'(x) = F(x), \quad y(1) = 0, \quad y(2) = 2, \tag{84}$$

where $F(x) = x^{3/2} \cos x$ has no closed-form integral of $\int_1^x F(s)ds$, such that $y(x)$ has also no closed-form solution. In this case we applied the Lie-group shooting method [14] to calculate $y$.

In Eq. (4) we require to know both $p(x_0)$ and $y'(x_0)$. This is a great drawback of the ND method. Because the calculated data of $y$ are discretized, we may approximate $y'(x_0)$ by $(y_1 - y_0)/\Delta x$. Then inserting the calculated data of $y$ into Eq. (4) we can obtain $p(x)$ by the ND method under $\sigma = 0$ and $\sigma = 0.001$, whose errors as shown in Fig. 6 are very large. The best parameter $\alpha$ is fixed to be 0.45 for $\sigma = 0$ and 0.43 for $\sigma = 0.001$.

Then, we apply Eq. (61) on this estimation of $p(x)$ by using $\Delta x = 0.01$ and $T = 0.01$, of which the errors under $\sigma = 0$ and $\sigma = 0.02$ are shown in Fig. 6. The errors of LGEM are much smaller than that obtained by the ND method with a ratio $10^{-4}$ of these two maximum errors for the un-noised case and $6.7 \times 10^{-3}$ for the noised case.

## 7 Conclusions

In order to estimate the potential function under a given spectral function and its corresponding eigenvalue, we have employed the LGEM to derive an algebraic equation and solved it in a closed-form. We transformed the inverse Sturm-Liouville problem into a parameter identification problem for a parabolic type PDE, and then, established a one-step GPS for the semi-discretization of that PDE. We also established an iterative method to estimate the unknown coefficient in a second-order Sturm-Liouville operator.

Numerical examples were worked out, which show that the new LGEM is applicable for the estimations of unknown functions. When disturbances are exerted on the input data we also verified that the present approach can be against them very well. The tested case shows that the LGEM is superior than the ND method examined here. Through this study, it can be concluded that the new estimation method is accurate, effective and stable. Its numerical implementation is very simple and the computational speed is very fast.

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Captions:

Fig. 1. For Example 1 of identifying the Schrödinger equation (a) plotting the estimation error by using the second spectral function, while (b) by using the third spectral function.

Fig. 2. For Example 2 of identifying $q(x)$ the estimation errors were plotted.

Fig. 3. For Example 3 by using an iterative method: (a) comparing estimated and exact $p(x)$, and (b) plotting the relative error of estimation.

Fig. 4. For Example 4 we compare exact $p(x)$ with the estimated ones by using an iterative method and a closed-form method.

Fig. 5. For Example 5 comparing the estimation errors of $p(x)$: (a) definite disturbances with $\delta = 0, 0.02$, and (b) random disturbance with $\sigma = 0.001$.

Fig. 6. For Example 6 comparing the estimation errors of $p(x)$ under random disturbances with $\sigma = 0$ and $\sigma = 0.001$.
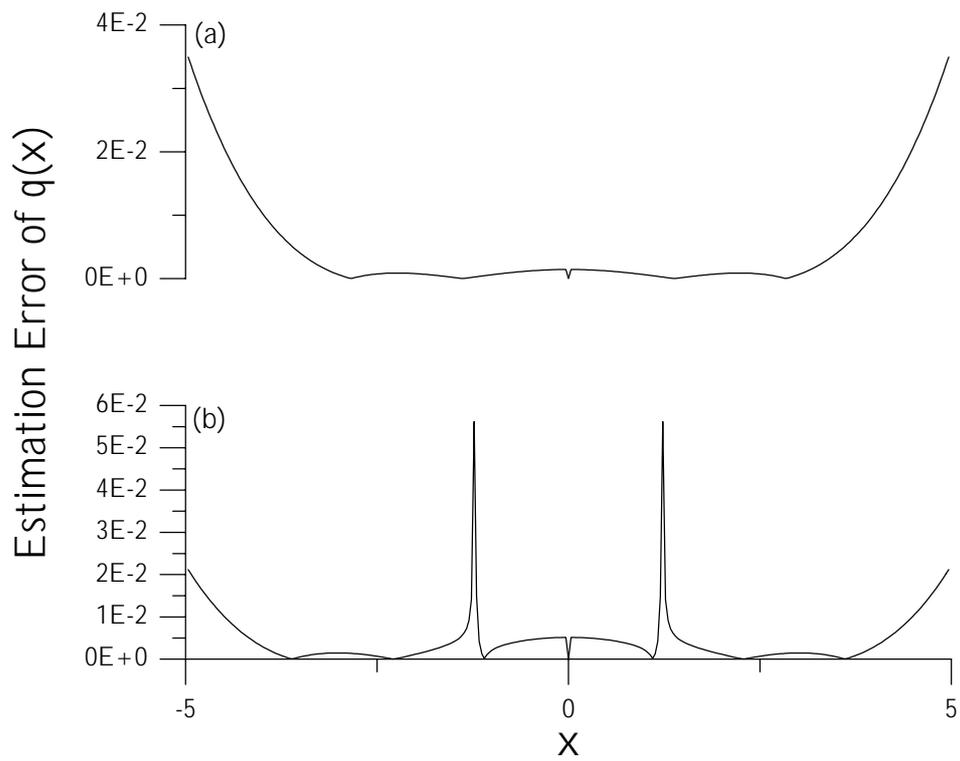
Fig. 1. For Example 1 of identifying the Schrodinger equation (a) plotting the estimation error by using the second spectral function, while (b) by using the third spectral function.
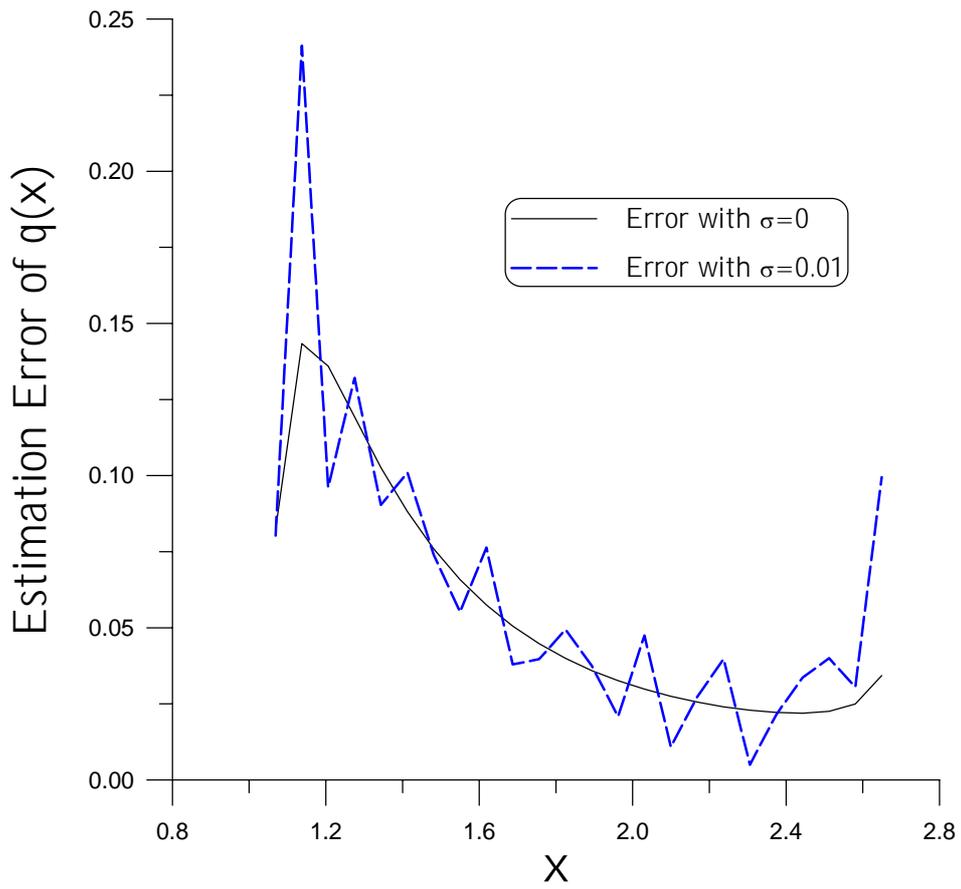
Fig. 2. For Example 2 of identifying q(x) the estimation errors were plotted.
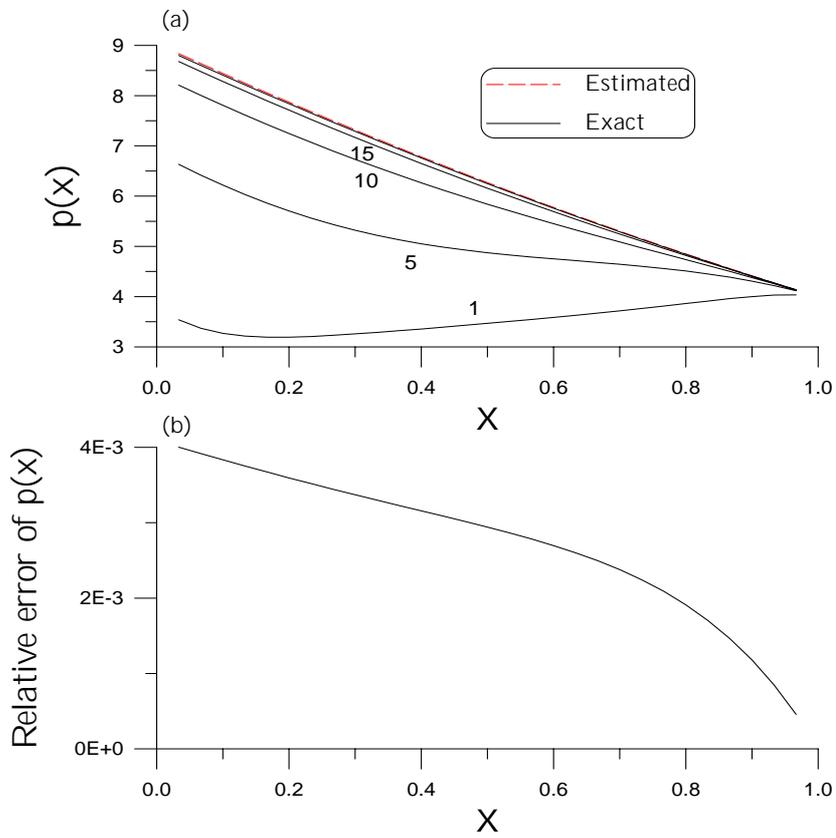
Fig. 3. Example 3 using an iterative method: (a) comparing estimated and exact p(x), and (b) plotting the relative error of estimation.
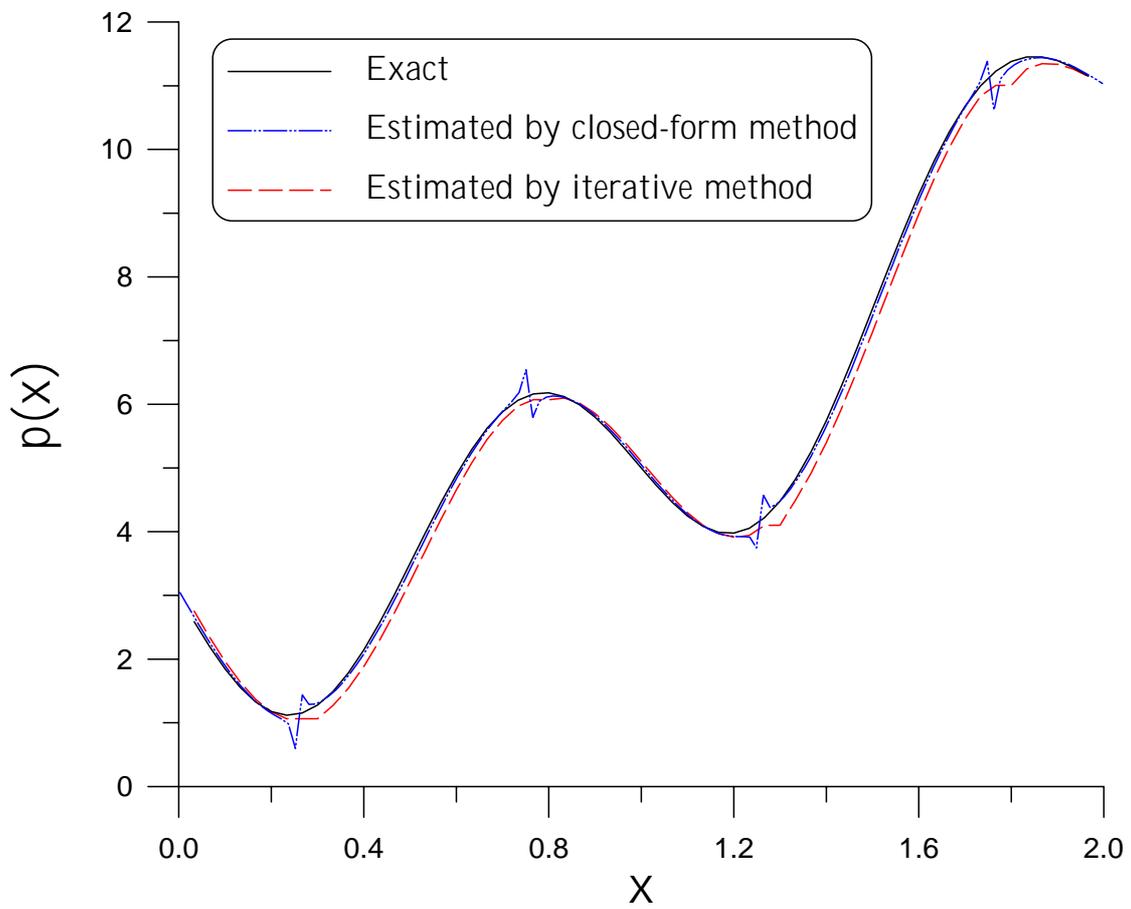
Fig. 4. Example 4 comparing exact p(x) with the estimated ones by using an iterative method and a closed-form method.

Fig. 5. For Example 5 comparing the estimation errors of p(x): (a) definite disturbances with  =0, 0.02, and (b) random disturbance with  =0.001.

Fig. 6. For Example 6 comparing the estimation errors of p(x) under random disturbances with    =0 and    =0.001.