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Derivative-Free Broyden's Method for Inverse Partially Known Sturm-Liouville Potential Functions

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Abstract : In this research a general potential function is recovered by the information of not only a set of equispaced nodes on half its domain but also a sequence of given eigenvalues. Furthermore in each iteration step Numerov's method is the main tool used to approximate the eigenvalues. In order to achieve our aim derivative-free Broyden's method is applied to solve a system of nonlinear equations. Additionally, the numerical implementation demonstrates that our method provides agreeable results.

Keywords : Inverse Sturm-Liouville problem; General symmetric potential; Numerov's method; Partially known potential function
2010 Mathematics Subject Classification : 65L09; 65L10;65L15;65F15;65F18.

1 Introduction

The second order ordinary differential equations are the core topic in the theory of differential equations and with several numerical techniques to reach solutions. One of the important topics in the second order differential equation is Sturm-Liouville problem (SLP) since it is one of the basic technique to solve solutions of partial differential equations. Moreover there are several mathematical model represented in the SLP such as in mechanical system the vibrational modes of

a string or sound waves in a pipe. Furthermore in quantum mechanics the SLP describes the time-independent Schödinger wave equation in one space dimension.

It is well-known that the general Sturm-Liouville equations can be rewritten as standard (regular,or Schrödinger) form

$$-y'' + qy = \lambda y, \qquad x \in (0, \pi) \tag{1.1}$$

with separated, self-adjoint boundary conditions

$$y'(0) - hy(0) = 0 \ \text{ and } \ y'(\pi) + Hy(\pi) = 0. \tag{1.2}$$

The impedance constants h and H are allowed to be real numbers and ∞. There are two extreme but common types of boundary conditions which are Dirichlet boundary condition ($h = \infty$) and Neumann boundary condition ($h = 0$). The function $q \in L^2[0, \pi]$ is called a potential function which is assumed to be real and piecewise continuous on $[0, \pi]$. The eigenvalues λ's are real, simple, countable and tend to infinity. Furthermore an infinite sequence of eigenvalues $\{\lambda_i\}_{i=1}^{\infty}$ is bounded from below by a constant a, i.e.

$$a < \lambda_1 < \lambda_2 < ... < \lambda_i < ...$$

Moreover the function y_i is said to be the eigenfunction corresponding to λ_i.

The asymptotic form of those eigenvalue sequences [1] is

$$\lambda_i = a_i + \bar{q} + \alpha_i(q) \qquad \text{with} \quad \bar{q} = \frac{1}{\pi}\int_0^{\pi} q(x)\mathrm{d}x, \qquad i = 1, 2, ... \tag{1.3}$$

where $a_i = O(i^2)$ depends on the boundary conditions, e.g., $a_i = i^2$ for Dirichlet-Dirichlet boundary conditions and $\bar{q}$ is the mean value of q. While a_i is independent of q, the sequence $\{\alpha_i(q)\}_{i=1}^{\infty} \in \ell^2$ depends on the potential q. It holds $\alpha_i \to 0$ if $i \to \infty$ with faster convergence for smoother q. Therefore, the term α_i in (1.3) contains important information on q.

In the direct problem the information of a potential function q is provided to acquire eigenvalues and eigenfunctions. Various numerical techniques discretize this problem to a finite computable approximation, including finite difference method, the Numerov's method and the finite element method. The knowledge of the eigenvalue of the matrix is employed since there are various theories and techniques for examples QR factorization, power method, and Householder's transformation.

In order to obtain the enhanced result an asymptotic correction [2, 3] is employed. Asymptotic correction is necessary for such matrix methods due to the asymptotic discrepancy between the eigenvalues of (1.1) and the eigenvalues of the used approximating matrix and, in detail, is essential to avoid swamping the vital $\alpha_i(q)$ term in (1.3) by the difference between the leading terms in the asymptotic expansion of the eigenvalues (1.1) and its discrete approximations, see [4, 5].

On the other hand we also focus on the issue of determination the potential function which is employed the information of eigenvalues. Borg [6] has shown that in order to determine uniquely a general potential function two different sets

of eigenvalues are sufficient. Furthermore Gel'fand and Levitan [7] utilized the information of eigenvalues and norming constants, $||y_i||^2/y_i(0)^2$, to uniquely retrieve a general potential function. Hochstadt and Lieberman [8] have proven that a single spectrum and partially half known potential function points are sufficient to uniquely accomplish a potential function on its entire interval. Kammanee and Böckmann [9] have applied the Hochstadt and Lieberman's theorem to recover a general potential functions. In order to solve a nonlinear equation the modified Newton's method is the main means.

In this research we introduce a method to recover a general potential function on the entire interval which a set of eigenvalues and a set of the partially known potential function on either $[\frac{\pi}{2}, \pi]$ or $[0, \frac{\pi}{2}]$ are the main information. In order to obtain the general potential function the system of non-linear equation is solved by derivative-free Broyden's method. Moreover the end of this paper demonstrates the numerical implementations investigating several types of functions such as a smooth continuous function, a non-smooth continuous function and a discontinuous function.

2 Methodology of the Inverse Problems

In this study we apply the theorem of Hochstadt and Lieberman[8] in order to approximate a general potential function based on the information of one sequence of eigenvalues and one sequence of partial known potential function representative over half of its domain. To create an algorithm for retrieving a general potential function, the n exact eigenvalues $\{\lambda_i\}_{i=1}^n$ and n equispaced potential nodes on either $[0, \frac{\pi}{2}]$ or $[\frac{\pi}{2}, \pi]$, which are $\{q_1, q_2, ..., q_n\}$ or $\{q_{n+1}, q_{n+2}, ..., q_{2n}\}$ are presented. In order to transform a continues problem to a discrete space, we investigate an n-vector whose ith entry where $i = 1, 2, ..., n$ is a approximation of a potential node $q(ih)$ or $q((n+i)h)$ with $h = \frac{\pi}{2n+1}$.

In each iteration step the eigenvalues are approximated, the best option to approximate eigenvalues is Numerov's method due to the fact that the order of precision is order four. Furthermore the exact eigenvalues λ_i are approximated by Λ_i which is computed from

$$Au + BQu = \Lambda u \tag{2.1}$$

where $A = (a_{i,j})$ is a symmetric tri-diagonal $2n \times 2n$ matrix whose elements are $a_{i,i} = \frac{2}{h^2}$ and $a_{i,i+1} = a_{i+1,i} = -\frac{1}{h^2}$ and Q is a centrosymmetric diagonal $2n \times 2n$ matrix where

$$Q = \begin{cases} \text{diag}\big(q_1, q_2, ..., q_n, \widehat{q}_{n+1}, \widehat{q}_{n+2}, ..., \widehat{q}_{2n}\big); & \text{for q known in } [\frac{\pi}{2}, \pi] \\ \text{diag}\big(\widehat{q}_1, \widehat{q}_2, ..., \widehat{q}_n, q_{n+1}, q_{n+2}, ..., q_{2n}\big); & \text{for q known in } [0, \frac{\pi}{2}] \end{cases} \tag{2.2}$$

where $\widehat{q}_i$ is the given potential function. Moreover the matrix $B = I - A/12$ where I is the identity matrix.

In order to reduce error the asymptotic correction is the chief process. For example, if $q(x) = 0$ with Dirichlet boundary conditions, the exact eigenvalues are

$\lambda_i = i^2$ and the approximated eigenvalues are $\Lambda_i = \frac{4\sin(ih/2)}{h^2}$ but $\frac{\Lambda_i}{\lambda_i} = \frac{4}{\pi} + O(h)$ as $i \to N$, see [4]. The correction term which is applied to relegate the error from $O(i^6h^4)$ to $O(i^4h^5/\sin(ih))$ with $q \in C^4[0,\pi]$ is defined by

$$\varepsilon(i,h) = i^2 - \frac{12\sin^2(ih/2)}{h^2[3-\sin^2(ih/2)]}. \tag{2.3}$$

The foremost problem in this research is to solve the $n-$nonlinear equations in n unknown which is the zero map $F : \mathbb{R}^n \to \mathbb{R}^n$ defined by

$$F(q) = \begin{pmatrix} \Lambda_1 - \widetilde{\lambda}_1 \\ \vdots \\ \Lambda_n - \widetilde{\lambda}_n \end{pmatrix} = \mathbf{0}. \tag{2.4}$$

Due to above reason first we have to make translation $\widetilde{\lambda}_i = \lambda_i - \varepsilon(i,h)$.

There are several researches such as [10, 11, 12] in this area applying the modified Newton's method (or fixed Jocobian Newton's method) to find the roots of the nonlinear equation (2.4) in order to avoid computationally heavy updating of the Jacobian matrix which is complicated. However in this paper we focus on the derivative-free Broyden's method, see [13, 14, 15] where the Jacobian matrix is approximated each iteration. However there is only the work of [16] utilizing the Broyden's method to solve inverse SLPs. The aim of research [16] is to recover general potential functions employing the information of two sequences of eigenvalues. Moreover the Broyden's method is the important numerical method to find the root of nonlinear equations.

Broyden's iteration is written as

$$A^{(k)}(q^{(k+1)} - q^{(k)}) = -F(q^{(k)}), \qquad k = 0, 1, ... \tag{2.5}$$

where $A^{(k)}$ is called the approximated updated Jacobian matrix which is defined as

$$A^{(k)} = A^{(k-1)} + UV^T, \tag{2.6}$$

with $V = q^{(k)} - q^{(k-1)}$ and $U = (VV^T)^{-1}(F(q^{(k)}) - F(q^{(k-1)}) - A^{(k-1)}V)$, see [13, 14, 15].

In order to achieve fast convergence we set $A^{(0)} = \Lambda'(q^{(0)})$. The matrix $A^{(0)}$ is the exact Jacobian whose (i,j)-th element $\Lambda_{i,j} = \dfrac{\partial \Lambda_i}{\partial q_j}$ is the partial derivative of $\Lambda_i(q^{(0)})$ with respect to q_j marked with the subscript "$,j$". Our technique to compute $\Lambda'(q^{(0)})$ is similar to [11, 12]. We consider the eigenvalue problem

$$-Ay_i + BQy_i = \Lambda_i B y_i, \tag{2.7}$$

where y_i represents the right eigenvector to the eigenvalue Λ_i. Differentiating (2.7) with respect to q_j and since the constant matrices A and B are independent of q_j we obtain

$$-Ay_{i,j} + B(Q_{,j}y_i + Qy_{i,j}) = \Lambda_{i,j}By_i + \Lambda_i By_{i,j}.$$

Assuming B is invertible, multiplication with B^{-1} yields

$$-B^{-1}Ay_{i,j} + Q_{,j}y_i + Qy_{i,j} = \Lambda_{i,j}y_i + \Lambda_i y_{i,j}.$$

Note that our numerical examples indicate that the condition number of B is low. Here and throughout the rest of this section, let the vector norm denote the standard Euclidean norm and let $\langle\cdot,\cdot\rangle$ denote the stand inner product. Hence,

$$\langle -B^{-1}Ay_{i,j}, v_i\rangle + \langle Q_{,j}y_i + Qy_{i,j}, v_i\rangle = \langle \Lambda_{i,j}y_i, v_i\rangle + \langle \Lambda_i y_{i,j}, v_i\rangle,$$

where v_i is the left eigenvector corresponding to Λ_i defined by

$$-v_i^T A + v_i^T BQ = \Lambda_i v_i^T B. \tag{2.8}$$

Due to the fact that $-A + BQ$ is not a symmetric matrix, the left and right eigenvectors are different in general. Now we obtain

$$[A^{(0)}]_{ij} = \Lambda_{i,j} = \frac{\langle Q_{,j}y_i, v_i\rangle}{\langle y_i, v_i\rangle} = \frac{v_i^T Q_{,j}y_i}{v_i^T y_i}, \tag{2.9}$$

where $Q_{,j}$ is the $2N \times 2N$ diagonal matrix of which the only non-zero elements are $[Q_{,j}]_{j,j} = 1$ and $[Q_{,j}]_{2N+1-j,2N+1-j} = 1$.

Algorithm 2.1. *Computing a general discretized potential function q on uniformly spaced nodes from one given sequence of eigenvalues and a given sequence of partially known potentials.*

Input *Tolerance threshold ϵ, maximum number of iterations M, the first n given eigenvalues $\lambda_1, \lambda_2, ..., \lambda_n$ and partially known potential function either on $[0, \pi/2]$ or $[\pi/2, \pi]$.*

1. *Set $k = 1$ and $\delta = \epsilon + 1$.*
2. *Compute $q_i^{(0)} = \lambda_n - n^2$ for $i = 1, ..., n$.*
3. *Compute the corrected eigenvalues $\widetilde{\lambda}_i = \lambda_i - \varepsilon(i, h)$ where $\varepsilon(i, h)$ is obtained by (2.3) in setting $q \equiv 0$.*
4. *Compute the eigenvalues Λ_i and the left (v_i) and right (y_i) eigenvector using (2.8) and (2.7).*
5. *Compute $A^{(0)}$ using (2.9) and $q^{(1)}$ using (2.5).*
6. *Repeat until either $\delta < \epsilon$ or $k > M$*
   (a) *Compute the first N eigenvalue of (2.7).*
   (b) *Compute $F(q)$ in (2.4) and then compute $A^{(k)}$ using (2.6).*
   (c) *Compute $q^{(k+1)}$ using (2.5) and $\delta = \|q^{(k+1)} - q^{(k)}\|$.*
   (d) *Set $k = k + 1$.*

Output *k, δ and $q^{(k)}$.*

Theorem 2.1 (Convergence of Algorithm 2.1)**.** *Let $N > 1$. Assume that the eigenvalue of $-B^{-1}A + Q$ are simple for all k. Then, there exists a constant C such that the iteration (2.5) converges to a solution q^* of (2.4) if $\|q^* - q^{(0)}\| \leq C$.*

Proof. Let $\|\cdot\|$ be a norm on $\mathbb{R}^n$. Since $F : \mathbb{R}^n \to \mathbb{R}^n$ is a continuously differential operator and $F'(q)$ is analytic for all q, there exist a Lipschitz constant $K > 0$ and the solution $q^* \in \mathbb{R}^n$. Furthermore, $(F'(q^*))^{-1}$ is assumed to exist. Then we obtain

$$\|F'(q^*)^{-1}(F'(q) - F'(q^*))v\| \leq K\|q - q^*\|\|v\|$$

for q and $v \in \mathbb{R}^n$. Let $\theta \in (0, 1)$ and $C = \dfrac{1-\theta}{2-\theta}\left(\dfrac{\theta}{\theta+1}\right)\dfrac{1}{K}$. It now follows from the standard theory of Broyden's method, see [13], that the sequence $\{q^{(k)}\}_{k=1}^{\infty}$ converges to the solution q^* of $F(q) = 0$ as

$$\|q^{(k)} - q^*\| < \frac{\theta^k}{K}\left(\frac{1-\theta}{2-\theta}\right)\left(\frac{\theta}{\theta+1}\right) \leq \frac{\theta^k}{K} \qquad k = 1, 2, ...$$

□

Moreover a reasonable choice for an initial guess $q^{(0)}$ follows a suggestion of [11, 12], where all elements are assumed to be a constant of obtained from approximating $\overline{q} = \lambda_n - n^2$. This is motivated by the asymptotic expansion of eigenvalues, cf. (1.3).

3 Numerical experiments

In this section the Algorithm 2.1 is investigated for recovering general potential functions which are recovered on various type functions. For the first two examples the smooth continuous functions which are $q_1(x) = \cos 3x$ and $q_2(x) = (\exp(x) - x^2)/12$ are considered. The non-smooth continuous function and discontinuous function are $q_3(x) = |x^2 - 2|$ and

$$q_4(x) = \begin{cases} 3/2 & \text{for } \pi/4 \leq x < \pi/2 \\ 2 & \text{for } \pi/2 \leq x < 3\pi/2 \\ x & \text{elsewhere} \end{cases}$$

, respectively. For all examples in this paper we employ 40 exact eigenvalues and 40 partially known potential nodes on either $[0, \pi/2]$ or $[\pi/2, \pi]$. The exact eigenvalues are computed by MATSLISE software package [17]. Moreover the tolerance threshold ϵ was set to 0.00005.

Due to the fact that the convergent rate of derivative-free Broyden's method is between 1 and 2 which is better than with modified Newton's method used in [3, 2], our iteration step count will in comparison be smaller.

In order to increase the accuracy we can employ more eigenvalues or find another with high-precision direct methods to approximate eigenvalues [10].

Table 1: The table shows the norm of error ($\times 10^{-6}$) and k stands for the number of the iteration step.

function	known potential on $[0, \frac{\pi}{2}]$	known potential on $[\frac{\pi}{2}, \pi]$
q_1	1.54985 $(k = 6)$	1.46982 $(k = 6)$
q_2	4.93512 $(k = 5)$	5.00135 $(k = 5)$
q_3	9.42044 $(k = 9)$	9.13251 $(k = 9)$
q_4	10.66687 $(k = 10)$	10.75428 $(k = 10)$

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