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BVMs for computing Sturm–Liouville symmetric potentials ☆

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ABSTRACT

The paper deals with the numerical solution of inverse Sturm–Liouville problems with unknown potential symmetric over the interval $[0,\pi]$. The proposed method is based on the use of a family of Boundary Value Methods, obtained as a generalization of the Numerov scheme, aimed to the computation of an approximation of the potential belonging to a suitable function space of finite dimension. The accuracy and stability properties of the resulting procedure for particular choices of such function space are investigated. The reported numerical experiments put into evidence the competitiveness of the new method.

1. Introduction

Inverse Sturm–Liouville problems (SLPs) consist of recovering the potential $q(x) \in L^2[0,\pi]$ from

$$-y'' + q(x)y = \lambda y, \quad x \in [0,\pi], \tag{1}$$
$$a_1 y(0) - a_2 y'(0) = 0, \quad |a_1| + |a_2| \neq 0, \tag{2}$$
$$b_1 y(\pi) - b_2 y'(\pi) = 0, \quad |b_1| + |b_2| \neq 0, \tag{3}$$

and the knowledge of suitable spectral data. They play an important role in several areas such as geophysics, engineering and mathematical-physics. The research concerning the development of numerical techniques for the approximation of their solution represents therefore a very active and interesting field of investigation.

The existence and uniqueness of the solution of an inverse SLP has been proved for several formulations of it among which we quote:

- The *two-spectrum* problem characterized by the knowledge of two sets of eigenvalues $\{\lambda_k^{(j)}\}_{k=1}^{\infty}$, $j = 1, 2$, corresponding to two SLPs sharing the first boundary condition (2) (BC in the sequel) and differing for the second one (3), [1];
- The *spectral function data* problem where the input consists of one spectrum $\{\lambda_k\}_{k=1}^{\infty}$ and the ratios $\{\|y_k\|_2^2/y_k^2(0)\}_{k=1}^{\infty}$ or $\{\|y_k\|_2^2/(y_k'(0))^2\}_{k=1}^{\infty}$ in the case $a_2 \neq 0$ or $a_2 = 0$, respectively. Here y_k denotes the eigenfunction corresponding to λ_k, [2];
- The *endpoint data* problem occurring when the spectrum of the SLP subject to Dirichlet BCs is known together with the terminal velocities $\kappa_k = \log(|y_k'(\pi)|/|y_k'(0)|)$, $k = 1, 2, \ldots$, [3];
- The *symmetric* problem for which a potential q satisfying

$$q(x) = q(\pi - x), \tag{4}$$

for all $x \in [0,\pi]$, has to be reconstructed from the knowledge of one spectrum corresponding to symmetric BCs (i.e. $a_1 b_2 + a_2 b_1 = 0$), [1].

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The latter is the problem that we shall consider in this paper. It is known that, if $q \in L^2[0,\pi]$, the kth eigenvalue of (1)–(3) behaves asymptotically as

$$\lambda_k = \lambda_k(q) = \mu_k + \overline{q} + \delta_k(q), \tag{5}$$

where $\mu_k = O(k^2)$ depends only on the BCs of the SLP, $\overline{q} = \frac{1}{\pi}\int_0^\pi q(x)dx$ and $\{\delta_k(q)\}_{k=1}^\infty \in \ell^2$, [4]. This implies that, in addition to (4), the information concerning the variation of q for the symmetric problem are contained in the small terms $\delta_k(q)$.

Obviously, in the practice, the set of known eigenvalues is finite and usually consists of the first M ones. The matrix methods are therefore well-suited for the solution of inverse SLPs and among them the three-point scheme and the Numerov method are the most popular ones. In general, the matrix methods are based on the use of finite difference or finite element methods for the solution of ODEs over an assigned partition of $[0,\pi]$ frequently composed by:

$$x_i = ih, \quad i = 0, 1, \ldots, N+1, \quad h = \frac{\pi}{N+1}. \tag{6}$$

When applied for solving direct SLPs, such methods replace the continuous problem with a generalized matrix eigenvalue one of the form

$$A(q)\mathbf{y}^{(h)} = \lambda^{(h)} S(q)\mathbf{y}^{(h)}. \tag{7}$$

Here $\lambda^{(h)}$ is the approximation of one of the exact eigenvalues, $\mathbf{y}^{(h)}$ the corresponding numerical eigenfunction and the square matrices $A(q)$ and $S(q)$, besides the potential q, depend on the particular method and on the BCs of the SLP. As well-known the accuracy of the approximation $\lambda_k^{(h)}$ of λ_k deteriorates significantly for increasing values of the index k so that the discretization error of a matrix method inevitably swamps the term $\delta_k(q)$ in (5) with the exception of the first few indices. The application of the asymptotic (or algebraic) correction technique, introduced in [5,6] for the three-point formula and in [7–9] for the Numerov method, allows to greatly improve such eigenvalue estimates. It is based on the observation that the leading term in the discretization error is independent of the potential q. This has suggested to correct the estimate $\lambda_k^{(h)}$ by adding to it the term $\epsilon_k^{(h)} = \lambda_{k,0} - \lambda_{k,0}^{(h)}$ where $\lambda_{k,0}$ and $\lambda_{k,0}^{(h)}$ are the kth exact and numerical eigenvalues corresponding to the potential $q(x) \equiv 0$, respectively.

Among the first successful algorithms for the solution of symmetric inverse SLPs subject to Dirichlet BCs (DBCs from now on) we mention the ones proposed in [10–12]. In particular, the method in [12] used the three-point scheme for which the coefficient matrix $A(q)$ in (7) is symmetric and tridiagonal while $S(q)$ is the identity matrix. The number of meshpoints N in (6) was set equal to the number M of known eigenvalues so that $A(q)$ was of size M. An inverse matrix eigenvalue problem for a centrosymmetric $A(q)$ was then solved with the very important shrewdness, derived from the asymptotic correction technique, of taking $\lambda_k - \epsilon_k^{(h)}$ as kth reference eigenvalue instead of simply λ_k for each k. From the knowledge of $A(q)$ an approximation $\mathbf{q}_{in}^{(h)}$ of $\mathbf{q}_{in} = (q(x_1), q(x_2), \ldots, q(x_N))^T$ was then easily computed. The defect of this method, however, was the use of the entire numerical spectrum which even after the application of the asymptotic correction presents discretization error of order $O(1)$ in the largest eigenvalues.

A more reliable method for the same type of inverse SLP was then proposed in [13] which still used the three-point formula but involved only the first half of the computed numerical eigenvalues. In this case, in fact, N was set equal to $2M$ and the approximation $\mathbf{q}_{in}^{(h)}$ of $\mathbf{q}_{in}$ was computed by solving the system of nonlinear equations

$$\lambda_k^{(h)} - \lambda_k + \epsilon_k^{(h)} = 0, \quad k = 1, 2, \ldots, M, \tag{8}$$

where $\lambda_k^{(h)} = \lambda_k^{(h)}(q) = \lambda_k^{(h)}\left(\mathbf{q}_{in}^{(h)}\right)$ represents the kth eigenvalue of $A(q)$. By virtue of the symmetry condition (4), the constraint $\mathbf{q}_{in}^{(h)} = \widehat{J}\mathbf{q}_{in}^{(h)}$ was imposed on $\mathbf{q}_{in}^{(h)}$ where $\widehat{J}$ denotes the anti-identity matrix. The unknowns in (8) were therefore the first M entries of $\mathbf{q}_{in}^{(h)}$ and a modified Newton method was used for solving such system. The convergence properties of the latter method were also studied in details in [13] for q "sufficiently" close to a constant.

A similar approach for solving symmetric inverse SLPs has been considered in [14,15] where the Numerov method has been used in place of the three-point formula. Moreover, in [15] the treatment of the Neumann boundary conditions (NBCs in the sequel) has been discussed. It must be said that while this extension is straightforward for the three-point method, the same definitely does not happen for the Numerov one.

As final reference for the currently available numerical techniques for the problem under consideration, we mention the one recently proposed in [16]. In this case the continuous problem is reformulated as a system of first order ODEs and a family of Boundary Value Methods (BVMs) obtained from the Obrechkoff formulas in conjunction with the asymptotic correction technique is applied for the solution of the direct problem (see also [17,18]). The resulting generalized eigenvalue problem (7) has size $4M - 4$ with $N = 2M - 3$ and the Newton method is used for solving (8).

In this paper, for the solution of the symmetric inverse problem, we consider the application of the BVMs introduced in [19,20] for the direct one. These schemes are obtained as a generalization of the Numerov method and provide competitive results with respect to the latter improved with the asymptotic correction technique. Moreover, in [20] a compact formulation of the corresponding generalized eigenvalue problem (7) is given which covers all possible types of BCs (2) and (3). With respect to the methods in [13–16], a relevant difference of our procedure is constituted by the fact that we look for an approximation of the unknown potential of the form $q^{(h)}(x) = \phi(x, \mathbf{c}^{(h)})$ where, for any $\mathbf{c} = (c_1, c_2, \ldots, c_L)^T$, $\phi(x, \mathbf{c}) = \sum_{j=1}^L c_j\phi_j(x)$ being $\{\phi_j(x)\}_{j=1}^L$ a set of symmetric linearly independent functions. The chosen value of L usually depends on