Approximation of eigenvalues of Sturm-Liouville problems defined on a semi-infinite domain

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Abstract

In this paper, we describe how to approximate numerically the eigenvalues of a Sturm-Liouville problem defined on a semi-infinite interval. The key idea is to transform the problem in such a way as to compress the semi-infinite interval in a finite interval by applying a suitable change of the independent variable. Then, we approximate each derivative in the Sturm-Liouville equation thus obtained with finite difference schemes. Consequently, we convert the Sturm-Liouville problem into an algebraic eigenvalue problem. The numerical results of the experiments show that the proposed approach is promising.

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1. Introduction

We focus our study on a classical one-dimensional Sturm-Liouville equation

$$-\left(p(x)y'(x)\right)' + q(x)y(x) = \lambda\omega(x)y(x) \tag{1}$$

defined on the semi-infinite interval $(0,\infty)$ and subject to Dirichlet boundary conditions

$$y(0) = y(\infty) = 0. \tag{2}$$

Here the set of Sturm-Liouville coefficients $\{p, q, \omega\}$ has to satisfy the following minimal conditions: (i) $p, q, \omega : (0,\infty) \longrightarrow \mathbb{R}$, (ii) $p^{-1}, q, \omega \in L^1_{loc}(0,\infty)$, (iii) p and ω are positive almost everywhere,

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cfr. [1]. The problem of finding a complex number λ such that the boundary value problem (1)-(2) has a non-trivial solution is called Sturm-Liouville problem (SLP). The value λ is called an eigenvalue and the corresponding solution y is called an eigenfunction.

The analytical treatment of this problem is in general very difficult. For this reason, numerical treatments and therefore the choice of good numerical approximation methods are essential. To deal with this problem numerically, we must first deal with its semi-infinite interval and transform it into a finite interval. Many of the numerical techniques available in the literature are based on the so-called regularization. In this context, this means truncating the interval and solving the resulting problem. In [2] the interval $(0, \infty)$ is replaced by the finite interval $[\varepsilon, b^*]$ where ε is strictly positive and small and b^* is large. The considered SLP is then transformed into a regular problem posed on the finite interval (ε, b^*) with boundary conditions $y(\varepsilon) = y(b^*) = 0$. The accuracy of the computed eigenvalues strongly depends on the choice of the cutoff points ε and b^*. Concerning the choice of b^*, a generalization of the so-called WKB-approximation was proposed in [2]. In the case of a problem whose potential has a Coulomb-like tail, the authors proposed to impose suitably adapted boundary conditions at the right endpoint b^* which allowed a noticeable reduction of the size of b^*. In [3] the problem is first converted to one on a finite interval (a, b) by an appropriate change of variables, or bilinear or homographic transformation if necessary (these transformations leave the spectrum of the problem unchanged). Otherwise, placing the interval $[a_T, b_T]$ instead of (a, b) such that $a_T, b_T \in (a, b)$ be close enough to a and b respectively, allows the problem to be a regular, and it is expected to approximate the given problem on (a, b). After that, the problem on $[a_T, b_T]$ is converted with change of variables by Prüfer transformation from the unknowns y, py' to new unknowns ρ, θ. And after calculating an initial approximation of the eigenvalue, that is obtained by the so called JWKB formula is shown in [4], where the interval of integration in JWKB formula is defined by part of (a, b) for which the integrand is real, a special method presented also in [4] gives an appropriate equation and initial conditions satisfactory for that initial approximation, to determine the function θ, and thus to determine a truncated endpoints a_T and b_T.

In [5] and [6] a change of variable implicitly converts the interval $(0, \infty)$ into a finite interval (a, b). Two initial points $a_0 > a$ and $b_0 < b$ are chosen, so the problem on a regular interval $[a_0, b_0]$ is a truncated problem with some of artificial boundary conditions at $x = a_0$ and $x = b_0$ are imposed. The choice of a_0 and b_0 will generally depend on the index of the eigenvalue requested. The interval $[a_0, b_0]$ is covered by a uniform mesh and an initial approximation of the eigenvalue is computed by

Pruess piecewise-constant approximation on $[a_0, b_0]$. The author after that add to $[a_0, b_0]$ additional intervals $[a_1, a_0]$ and $[b_0, b_1]$ such that a_1 is obtained by stepping from a_0 towards a and similarly for b_1, and an additional eigenvalue approximation is computed on $[a_1, b_1]$. This process is repeated until some eigenvalue approximations agree with the tolerance specified by the user.

In [7], an initial mesh is constructed by equidistribution process depended on the coefficient functions p, q and w that is described in [8], the infinite endpoint corresponding to the last initial mesh subinterval is transformed to zero by the change of variable $t = -1/x$, and subsequent using midpoint interpolation to the first subinterval of the mesh in terms of x and to the last subinterval of the mesh in terms of t for truncating the interval at that midpoints and replacing the coefficient functions by step function approximations corresponding to this initial mesh is done to regularize the problem. This mesh is then bisected, which means united with its midpoints, to produce a new mesh, and these truncation points move closer to the singular endpoints every time the mesh is bisected. However, the boundary conditions are applied at the original endpoints, except at the infinite endpoint, it is replaced by a large number.

Another technique is presented in [9]. In this case, the interval $(0, \infty)$ is divided into two intervals $(0, 1]$ and $[1, \infty)$ and this second interval is transformed into $(0, 1]$ by a suitable change of the independent variable, namely $x \to 1/x$. The original problem in the semi-infinite interval $(0, \infty)$ is then transformed into a problem posed on the interval $(0, 1)$ but of double dimension. In fact, the first equation derives from the original problem defined on $(0, 1)$ while the second equation derives from the original problem on $(1, \infty)$ after changing the variable $x \to 1/x$. The boundary conditions must obviously also take into account the matching condition for the solution at $x = 1$. The technique of changing the variable is efficient and applicable even in the case of Sturm-Liouville problems with other boundary conditions on $(0, \infty)$, as shown in [10, 11]. However, doubling the size of the problem numerically leads to double the computational cost. To overcome this problem in [12, 13] for the numerical treatment of the radial Schrödinger eigenproblems two change of variable have been proposed which compress the interval $(0, \infty)$ directly to $(0, 1)$. They are described by the two functions

$$t_1(x) = x/(x + \alpha), \quad \alpha > 0, \qquad\qquad t_2(x) = 1 - (1 + x)^{-\beta}, \quad \beta > 0.$$

A good choice of the parameters α and β allows a good approximation of the solutions.

In this paper we propose a change of the independent variable for the transformation of the original Sturm-Liouville problem (1)-(2) on a finite domain. This is presented in Section 2. The remaining part of the paper is organized as follows. In Section 3 we describe the numerical schemes used for discretizing the continuous problem thus obtained and we analyze the order of accuracy of the eigenvalues estimates that these schemes provide. Section 4 contains the numerical results obtained on several examples considered. Finally, some conclusions are drawn is Section 5.

2. Reformulation of the problem on the interval $(0, 1)$

Our goal in this section is to identify a function that by modifying the independent variable can transform equation (1) into an equation with new coefficients, but which has the same eigenvalues over a finite interval. For this purpose, consider the function u defined by

$$u(x) = \frac{2}{\pi}\arctan(\phi x), \quad x \in [0, \infty), \tag{3}$$

where ϕ is a positive real parameter. Setting $\tilde{x} = u(x)$, it is immediate to derive that $y(x) = y(u^{-1}(\tilde{x}))$. Then, by posing $z(\tilde{x}) := y(x)$ we can rewrite the equation (1) as

$$-\frac{d}{dx}\left(p(x)\frac{d}{dx}u(x)\frac{d}{d\tilde{x}}z(\tilde{x})\right) + q(x)z(\tilde{x}) = \lambda\omega(x)z(\tilde{x}). \tag{4}$$

Consequently, since $x = u^{-1}(\tilde{x})$, we obtain

$$-\frac{d}{d\tilde{x}}\left(\frac{1}{\frac{d}{d\tilde{x}}u^{-1}(\tilde{x})}p(u^{-1}(\tilde{x}))\frac{d}{d\tilde{x}}z(\tilde{x})\right) + \frac{d}{d\tilde{x}}u^{-1}(\tilde{x})q(u^{-1}(\tilde{x}))z(\tilde{x}) = \lambda\frac{d}{d\tilde{x}}u^{-1}(\tilde{x})\omega(u^{-1}(\tilde{x}))z(\tilde{x}). \tag{5}$$

Now, recalling that $\tilde{x} = u(x)$, from (3) we deduce that

$$x = \frac{1}{\phi}\tan\left(\frac{\pi}{2}\tilde{x}\right).$$

Finally, by using this relation in (5) we get the Sturm-Liouville equation transformed as follows

$$-\frac{d}{d\tilde{x}}\left(\tilde{p}(\tilde{x})\frac{d}{d\tilde{x}}z(\tilde{x})\right) + \tilde{q}(\tilde{x})z(\tilde{x}) = \lambda\tilde{\omega}(\tilde{x})z(\tilde{x}), \tag{6}$$

where

$$\tilde{p}(\tilde{x}) = \frac{2\phi}{\pi}\cos^2\left(\frac{\pi}{2}\tilde{x}\right)\ p\left(\frac{1}{\phi}\tan\left(\frac{\pi}{2}\tilde{x}\right)\right), \tag{7}$$

$$\tilde{q}(\tilde{x}) = \frac{\pi}{2\phi}\sec^2\left(\frac{\pi}{2}\tilde{x}\right)\ q\left(\frac{1}{\phi}\tan\left(\frac{\pi}{2}\tilde{x}\right)\right), \tag{8}$$

$$\tilde{\omega}(\tilde{x}) = \frac{\pi}{2\phi}\sec^2\left(\frac{\pi}{2}\tilde{x}\right)\ \omega\left(\frac{1}{\phi}\tan\left(\frac{\pi}{2}\tilde{x}\right)\right). \tag{9}$$

In this context, the boundary conditions (2) are transformed to

$$z(0) = z(1) = 0. \tag{10}$$

Obviously, the problem (6)–(10) is a Sturm-Liouville problem with singularity at one or two endpoints. Nevertheless, there are numerical methods that can handle this kind of problems. However, it is worth mentioning that there are some shooting approximation methods which cannot be used for dealing with our transformed problem. This is because these methods are constructed only to deal with equations in *Liouville normal form*, that is achieved via the Liouville's transformation, see [14, 15] for more details, which in general is not our case.

3. High order finite difference schemes

In this section we describe the main feature of the finite difference schemes we have used for solving the SLP reformulated on the finite interval $(0, 1)$. Before that, we write the problem (6)–(10) in the following form:

$$a_2(\tilde{x})z''(\tilde{x}) + a_1(\tilde{x})z'(\tilde{x}) + a_0(\tilde{x})z(\tilde{x}) = \lambda z(\tilde{x}), \tag{11}$$

$$z(0) = z(1) = 0, \tag{12}$$

where

$$a_2 = -\frac{\tilde{p}}{\tilde{\omega}}, \qquad a_1 = -\frac{\tilde{p}'}{\tilde{\omega}}, \qquad a_0 = \frac{\tilde{q}}{\tilde{\omega}} \tag{13}$$

and suppose that it admits a unique solution $z(\tilde{x})$ for $\tilde{x} \in [0, 1]$. Then, we introduce an equispaced grid

$$\tilde{x}_i = ih, \quad i = 0, 1, \ldots, N + 1, \quad h = \frac{1}{N + 1} \tag{14}$$

for the interval $[0, 1]$. The methods that we will consider allow us to discretize directly the problem in its second order formulation. They have been introduced in [16] and already used for the numerical solution of SLPs in [12, 13, 17]. The idea on which they are based is to approximate the first and second derivative at the inner grid points by applying suitable $(2k)$-step finite difference schemes. In more details, for $i = k, k + 1, \ldots, N + 1 - k$,

$$z^{(\nu)}(\tilde{x}_i) \approx \frac{1}{h^\nu} \sum_{j=0}^{2k} \delta_{k,j}^{(\nu)} z_{i+j-k}, \qquad \nu = 1, 2, \tag{15}$$

where $z_i \approx z(\tilde{x}_i)$ and, for each fixed value of ν, the coefficients $\{\delta_{k,j}^{(\nu)}\}_{j=0}^{2k}$ are uniquely determined by requiring the formula to have maximum order of consistency, i.e. $2k$. For $k \geq 2$, these formulas should be used together with the following formulas which provide approximations of the derivatives in the initial and final points of the mesh and are called *initial* and *final schemes*. In particular, for $i = 1, 2, \ldots, k-1$,

$$z^{(\nu)}(\tilde{x}_i) \approx \frac{1}{h^\nu} \sum_{j=0}^{2k+\nu-1} \delta_{i,j}^{(\nu)} z_j, \qquad \nu = 1, 2, \tag{16}$$

while, for $i = N + 2 - k, \ldots, N$,

$$z^{(\nu)}(\tilde{x}_i) \approx \frac{1}{h^\nu} \sum_{j=0}^{2k+\nu-1} \delta_{i-s,j}^{(\nu)} z_{j+s+1-\nu}, \qquad \nu = 1, 2, \quad s = N + 1 - 2k. \tag{17}$$

The coefficients occurring in (16) and (17) are determined by imposing the formulas to be of consistency order $2k$.

By applying the discretizations (15), (16) and (17) to the equation (11), we obtain the following algebraic eigenvalue system:

$$(A_2\Delta_2 + A_1\Delta_1 + A_0\Delta_0)\hat{Z} = \lambda\hat{Z}.$$

Here, for $\mu = 0, 1, 2$, A_μ denotes the diagonal matrix of size N whose non zero entries are given by $(A_\mu)_{ii} = a_\mu(\tilde{x}_i)$, $i = 1, 2, \ldots, N$ (see (13)), Δ_μ are real matrices of size $N \times (N+2)$ which contain the coefficients $\delta_{i,j}^{(\mu)}/h^\mu$ and $\hat{Z} = (z_0, z_1, \ldots, z_N, z_{N+1})^T \equiv (z_0, Z^T, z_{N+1})^T$.

To deal with the singularities at $\tilde{x}_0 = 0$ and $\tilde{x}_{N+1} = 1$, it is sufficient to use the boundary conditions $z(\tilde{x}_0) = 0$ and $z(\tilde{x}_{N+1}) = 0$. Consequently, we should eliminate the first and last column of the matrices Δ_ν thus obtaining matrices $\hat{\Delta}_\nu$ of size N and the well-defined eigenvalue problem

$$\hat{R}Z := (A_2\hat{\Delta}_2 + A_1\hat{\Delta}_1 + A_0)Z = \lambda Z. \tag{18}$$

Therefore, the eigenvalues of (11) are computed by the eigenvalues of the sparse banded matrix $\hat{R}$, see [17] for more details.

Before to conclude this section we explain how the coefficients $\delta_{i,j}^{(\nu)}/h^\nu$ in (15), (16) and (17) can be computed. For symmetry reasons, we only need to consider the first k formulas, i.e. $i = 1, 2, \ldots, k$. Therefore, we focus on the first grid points $\tilde{x}_j$, $j = 0, 1, \ldots, r$, with $r > k$. For any integer ℓ, setting $\Omega_\ell(\tilde{x}) = \prod_{s=0}^{\ell}(\tilde{x} - \tilde{x}_s)$, we denote by

$$F_{r,j}(\tilde{x}) = \frac{\Omega_r(\tilde{x})}{\Omega_r'(\tilde{x}_j)(\tilde{x} - \tilde{x}_j)} \tag{19}$$

the jth polynomial in the Lagrange basis. As it is well-known, $F_{r,j}(\tilde{x}_i)$ takes the value 0 at $i \neq j$ and 1 at $i = j$. Then, the Lagrange interpolation polynomial based on the first $r+1$ function values $z(\tilde{x}_j)$ becomes

$$\rho(\tilde{x}) = \sum_{j=0}^{r} F_{r,j}(\tilde{x}) z(\tilde{x}_j). \tag{20}$$

Therefore, by approximating the function z by the polynomial ρ we get the following relations

$$\frac{d^\nu}{d\tilde{x}^\nu} z(\tilde{x}) \approx \frac{d^\nu}{d\tilde{x}^\nu} \rho(\tilde{x}) = \sum_{j=0}^{r} \frac{d^\nu}{d\tilde{x}^\nu} F_{r,j}(\tilde{x}) z(\tilde{x}_j), \quad \nu = 1, 2. \tag{21}$$

The equation (19) implies the recursion relations

$$\begin{aligned} F_{r,j}(\tilde{x}) &= \frac{\tilde{x} - \tilde{x}_r}{\tilde{x}_j - \tilde{x}_r} F_{r-1,j}(\tilde{x}), \qquad j = 0, 1, \ldots, r-1, \\ F_{r,r}(\tilde{x}) &= \frac{\Omega_{r-2}(\tilde{x}_{r-1})}{\Omega_{r-1}(\tilde{x}_r)} (\tilde{x} - \tilde{x}_{r-1}) F_{r-1,r-1}(\tilde{x}). \end{aligned}$$

We differentiate all the above relations and evaluate them at $\tilde{x} = \tilde{x_i}, i = 1, 2, \ldots, k$. Denoting by

$$\delta_{i,j,r}^{(\nu)} = \frac{d^\nu}{d\tilde{x}^\nu} F_{r,j}(\tilde{x_i}), \quad \nu = 1, 2, \tag{22}$$

they can be written as follows

$$\delta_{i,j,r}^{(\nu)} = \frac{1}{\tilde{x}_j - \tilde{x}_r} \left(\nu \, \delta_{i,j,r-1}^{(\nu-1)} + (\tilde{x}_i - \tilde{x}_r) \, \delta_{i,j,r-1}^{(\nu)} \right), \quad j = 0, 1, \ldots, r-1, \tag{23}$$

$$\delta_{i,r,r}^{(\nu)} = \frac{\Omega_{r-2}(\tilde{x}_{r-1})}{\Omega_{r-1}(\tilde{x}_r)} \left(\nu \, \delta_{i,r-1,r-1}^{(\nu-1)} + (\tilde{x}_i - \tilde{x}_{r-1}) \, \delta_{i,r-1,r-1}^{(\nu)} \right). \tag{24}$$

Considering that $\delta_{i,j,1}^{(2)} = 0$ for each positive integer i, given the initial coefficients $\delta_{i,j,1}^{(1)}$ these recursion relations allow to determine all the coefficients $\{\delta_{i,j,r}^{(\nu)}\}_{j=0}^{r}$.

The recursion relations (23)-(24) constitute the algorithm proposed by Fornberg in [18, 19]. Although these coefficients of the considered numerical schemes can be computed also by solving Vandermonde linear systems, due to the ill-conditioning here we have preferred to use the Fornberg algorithm which is numerically short, fast and stable, cf. [20]. Furthermore, we note that this algorithm is also valid for irregular grid spacing.

From (21) and (22) we have that the coefficients in (15) are obtained when we set $r = 2k$ and $i = k$ in (23)-(24), namely

$$\frac{1}{h^\nu} \delta_{k,j}^{(\nu)} := \delta_{k,j,2k}^{(\nu)}, \qquad j = 0, 1, \ldots, 2k.$$

Instead, for $i = 1, 2, \ldots, k-1$, the coefficients characterizing formulas (16) are obtained by fixing $r = 2k + \nu - 1$, i.e.

$$\frac{1}{h^\nu}\delta_{i,j}^{(\nu)} := \delta_{i,j,2k+\nu-1}^{(\nu)}, \qquad j = 0, 1, \ldots, 2k + \nu - 1.$$

3.1. Convergence analysis

As just showed, we replace the SLP (11)-(12) by a matrix eigenvalue problem

$$\hat{R}Z = \lambda Z,$$

(see (18)). Defining by $\mathbf{z}$ the vector of values of z at the meshpoints, i.e.,

$$(\mathbf{z})_j = z(jh), \qquad j = 1, 2, \ldots, N,$$

we can define the local truncation error $\boldsymbol{\tau}$ by

$$\boldsymbol{\tau} = \hat{R}\,\mathbf{z} - \lambda\,\mathbf{z}.$$

When $\hat{R}$ is symmetric, as pointed out by Keller in [21, Theorem 1], the quality of the eigenvalue approximations will be proportional to the local truncation error. However, when we use $(2k)$-step finite difference schemes with $k \geq 2$, the matrix $\hat{R}$ loses its symmetry structure and therefore, this result cannot be applied. Anyway, considering that in these cases $\hat{R}$ can be read as a symmetric matrix plus a low rank matrix whose norm is independent of N and that $\hat{R}$ is a consistent discretization of the SLP having simple eigenvalues, it seems reasonable to assume that $\hat{R}$ is diagonalizable. Following the analysis carried out in [22] a basic result on approximating the eigenvalues of (11)-(12) by those of (18) can now be stated as

Theorem 1. *Let U be the matrix of eigenvectors of $\hat{R}$ normalized to be of unit length. Let $\boldsymbol{\tau}$ be the local truncation error as above and λ^* the eigenvalue corresponding to the eigenfunction z. Then*

$$|\lambda^* - \lambda| = \inf_{\mu \in \sigma(\hat{R})} |\lambda^* - \mu| \leqslant \mathrm{cond}(U)\frac{\|\boldsymbol{\tau}\|}{\|\mathbf{z}\|}, \tag{25}$$

where $\sigma(\hat{R})$ denotes the spectrum of $\hat{R}$ and $\mathrm{cond}(U)$ is the condition number of U.

This result shows that if the condition number of U can be bounded independently of h, then any eigenvalue of the SLP (11)-(12) will be approximated with an error which depends on the local

truncation error associated to the numerical scheme used and with the exact eigenfunction. In practice, it is rather difficult to prove *a priori* bounds on cond(U), but if one is interested in some fixed finite h, cond(U) can then be estimated numerically. Consequently, from Theorem 1 it follows that there exists a constant C independent of h and of the index i of the eigenvalue such that

$$|\lambda_i^* - \lambda_i| \leqslant C \frac{\|\boldsymbol{\tau}_i\|_2}{\|\mathbf{z}_i\|_2}.$$

Here $\mathbf{z}_i$ is the projection of the ith eigenfunction over the uniform mesh and $\boldsymbol{\tau}_i$ is the corresponding local truncation error. The reader may object that this result is not usable because it involves the vector $\mathbf{z}_i$ of values in the meshpoints of the unknown eigenfunction. However, although a rough approximation can be given by the right eigenvector of $\hat{R}$ corresponding to λ_i (see [22, Remark 2] for further details), from [23, Lemma 2.1] we know that when the Sturm-Liouville eigenvalue problem reduces to the study of the canonical Liouville normal form the ith eigenfunction satisfies

$$z_i(\tilde{x}) = \sin(i\pi\tilde{x}) + e(\pi\tilde{x})$$

where $e^{(\ell)}(\pi\tilde{x}) \sim O(i^{\ell-1}), \ell = 0, 1, 2, \ldots$ (here the superscript denotes the ℓth order differentiation w.r.t. $\tilde{x}$). In particular, this implies that $\|\sqrt{h}\mathbf{z}_i\|_2 \sim O(1)$. In addition, it allows to study the behavior of the associated local truncation error. In fact, in this context the jth component of $\boldsymbol{\tau}_i$ satisfies

$$|\tau_j| \leq |\gamma_j| \, (i\pi)^{\rho+1} h^{\rho-1} |\cos(i\pi\xi_j)| + O(i^\rho h^{\rho-1}), \quad j = 1, 2, \ldots, N, \tag{26}$$

where $\rho = 2k$ and γ_j is the principal error coefficient of the jth formula. The vector $\boldsymbol{\tau}_i$ can be split as $\boldsymbol{\tau}_i = \boldsymbol{\tau}_i^{(a)} + \boldsymbol{\tau}_i^{(m)}$, with $\boldsymbol{\tau}_i^{(a)} = (\tau_1, \ldots, \tau_{k-1}, 0, \ldots, 0, \tau_{N-k+2}, \ldots, \tau_N)^T$. By considering that the number of nonzero entries of such vector is independent of N (or, equivalently, of h), one has

$$\|\sqrt{h}\boldsymbol{\tau}_i\|_2 \leq \|\sqrt{h}\boldsymbol{\tau}_i^{(a)}\|_2 + \|\sqrt{h}\boldsymbol{\tau}_i^{(m)}\|_2 \sim O\left(i^{\rho+1}h^{\rho-1/2}\right) + O\left(i^{\rho+1}h^{\rho-1}\right).$$

The above considerations can be summarized in the following result.

Theorem 2. *Let λ_i^* the ith exact eigenvalue of the SLP in Liouville normal form and λ_i be the corresponding numerical eigenvalue provided by the $(2k)$-step finite difference scheme (15)–(17), with $k \geq 1$. Moreover, let U be as in Theorem 1. If* cond(U) *is bounded independently of N in Euclidean norm, and if (ih) is sufficiently small, then*

$$|\lambda_i - \lambda_i^*| \sim O\left(i^{\rho+1}h^{\rho-1/2}\right) + O\left(i^{\rho+1}h^{\rho-1}\right), \qquad \rho = 2k. \tag{27}$$

For any fixed i, the eigenvalue λ_i^* can be approximated to arbitrary accuracy by taking h sufficiently small. In practice, however, this can be computationally demanding when the index i becomes large. In these cases, the matrix approach we have proposed can be used to generate a set of eigenvalues with moderate accuracy which serves as starting values for well-established codes for the solution of SLPs as, for example, the `MATLAB` code `bvpsuite` based on a collocation method on adaptive meshes with reliable error control [24, 25]. Alternatively, to improve the efficiency of the proposed matrix approach, an adaptive step-size selection strategy could be implemented, but this will not be considered in this paper.

4. Numerical tests

To examine the performance of the proposed approach we now consider four examples of SLPs defined on a semi-infinite interval and with Dirichlet boundary conditions.

In all our experiments we have fixed the parameter ϕ in (3) depending on the index of the eigenvalues i

$$\phi = 0.6\,(i+1)^{-0.7}, \qquad i \in \mathbb{N},$$

and we have computed the eigenvalues using the `Matlab` function `eig`.

Example 1 Consider the Whittaker differential equation,

$$-y''(x) + \left(\frac{1}{4} + \frac{\kappa^2 - 1}{x^2}\right) y(x) = \lambda \frac{1}{x} y(x), \qquad x \in (0, \infty) \tag{28}$$

where the parameter $\kappa \geq 1$. When it is combined with boundary conditions $y(0) = y(\infty) = 0$, the eigenvalues are explicitly given by

$$\lambda_i^* = i + \frac{\kappa + 1}{2}, \quad i \in \mathbb{N}. \tag{29}$$

This differential problem is selected from [26] and studied in [27].

Applying the change of variable (3) to the equation (28) we get

$$-\frac{4\phi}{\pi^2}\cos^4(\frac{\pi}{2}\tilde{x})\tan(\frac{\pi}{2}\tilde{x})z''(\tilde{x}) + \frac{4\phi}{\pi}\cos^3(\frac{\pi}{2}\tilde{x})\sin(\frac{\pi}{2}\tilde{x})\tan(\frac{\pi}{2}\tilde{x})z'(\tilde{x}) + \left(\frac{1}{4\phi}\tan(\frac{\pi}{2}\tilde{x}) + \frac{\phi(\kappa^2-1)}{\tan(\frac{\pi}{2}\tilde{x})}\right) z(\tilde{x}) = \lambda z(\tilde{x}), \tag{30}$$

for all $\tilde{x} \in (0, 1)$.

We solve the corresponding SLP subject to Dirichlet boundary conditions using $2k$-step finite difference schemes for $k = 1, 2, 3, 4$ (of order $2, 4, 6, 8$, respectively), as explained in Section 3.

$i = 0, \lambda_0^* = 1$								
N	order 2	rel. err.	order 4	rel. err.	order 6	rel. err.	order 8	rel. err.
100	0.9999756431	2.4357e-05	0.9999997429	2.5709e-07	0.9999999953	4.7132e-09	0.9999999997	2.8510e-10
150	0.999989104	1.0896e-05	0.9999999482	5.1829e-08	0.9999999996	4.3523e-10	1.0	1.2621e-11
300	0.999997258	2.7420e-06	0.9999999967	3.2959e-09	1.0	5.9981e-12	1.0	6.5581e-13
$i = 1, \lambda_1^* = 2$								
100	1.999890214	5.4893e-05	1.999999047	4.7646e-07	1.999999988	6.1242e-09	1.999999999	2.5074e-10
150	1.999950923	2.4539e-05	1.999999807	9.6627e-08	1.999999999	5.6176e-10	2.0	1.0838e-11
300	1.999987655	6.1724e-06	1.999999988	6.1726e-09	2.0	9.1330e-12	2.0	4.9405e-14
$i = 2, \lambda_2^* = 3$								
100	2.999589756	1.3675e-04	2.999996607	1.1309e-06	2.999999957	1.4285e-08	2.999999998	5.3934e-10
150	2.999816702	6.1099e-05	2.999999299	2.3351e-07	2.999999996	1.3224e-09	3.0	2.2890e-11
300	2.999953908	1.5364e-05	2.999999955	1.5102e-08	3.0	2.1414e-11	3.0	3.4224e-13
$i = 13, \lambda_{13}^* = 14$								
100	13.90682566	0.0067	14.01453637	0.0010	14.00198871	1.4205e-04	14.00017176	1.2269e-05
150	13.9589175	0.0029	14.00244954	1.7497e-04	14.00013208	9.4343e-06	14.00000534	3.8142e-07
300	13.98974998	7.3214e-04	14.00003185	2.2753e-06	14.00000038	2.7013e-08	14.0	1.8334e-10

Table 1: Computed eigenvalues for Example 1, using the methods of order 2,4,6,8 and several values of N.

Table 1 lists the approximations of the eigenvalues $\lambda_i^*, i = 0, 1, 2, 13$ of the Whittaker problem for $\kappa = 1$ obtained for different values of N. In addition, the relative error is also reported for each case.

The most remarkable advantage of the proposed approach is the high accuracy: the higher order method and the small constant stepsize allow to compute more accurate solutions.

Example 2 Let us now consider the Half-range anharmonic oscillator equation,

$$-y''(x) + x^\alpha y(x) = \lambda y(x), \qquad x \in (0, \infty). \tag{31}$$

This differential equation is studied in [28] and when the parameter $\alpha = 2$ the exact eigenvalues are known to be

$$\lambda_i^* = 4i + 3, \quad i \in \mathbb{N}. \tag{32}$$

This is an alternate eigenvalues of harmonic oscillator. Instead, for others value of α in our tests we consider as exact values the one reported in [1]. In particular,

- for $\alpha = 3$:

$$\lambda_0^* = 3.4505626899; \quad \lambda_{24}^* = 228.52088139; \tag{33}$$

- for $\alpha = 4$:

$$\lambda_0^* = 3.7996730298; \quad \lambda_{24}^* = 397.14132678; \tag{34}$$

- for $\alpha = 5$:

$$\lambda_0^* = 4.0891593149; \quad \lambda_{24}^* = 588.17824969. \tag{35}$$

In Table 2 the eigenvalue approximations computed with the method of order 8 have been listed and compared to those obtained by `Matslise 2.0`, which is an well-established `Matlab` software package for the numerical solution of Sturm-Liouville problems [29, 30]. In Table 3 the eigenvalue approximations computed with the method of order 8 have been compared to those reported in [1]. In all cases, the relative errors has been also calculated.

The analysis of the results presented in Tables 2-3 shows that, in order to obtain good approximations, the method of order 8 is effective especially for small values of i, and their effectiveness is reduced for large values of i. As result, minimizing the constant stepsize addresses that.

$\alpha = 2$						
i	λ_i^*	N	λ_i	rel. err.	Matslise	rel. err.
0	3	150	2.9999999999992308	2.5639e-13	3.000000015191716	5.0639e-09
1	7	150	6.9999999999960423	5.6539e-13	6.999999999940737	8.4663e-12
2	11	150	10.999999999834149	1.5077e-11	10.999999994212841	5.2580e-10
3	15	200	14.999999999761719	1.5885e-11	14.999999998937918	7.0805e-11
4	19	200	18.9999999984874	7.9611e-11	18.999999992592333	3.8988e-10
5	23	200	22.999999997234017	1.2026e-10	23.000000008609277	3.7432e-10
6	27	300	26.99999999802748	7.3056e-11	26.999999994713050	1.9584e-10
7	31	300	30.999999995128078	1.5716e-10	31.000000011928531	3.8479e-10
8	35	400	34.999999997116319	8.2391e-11	34.999999995608334	1.2548e-10
16	67	900	66.999999997183579	4.2036e-11	66.999999996702115	4.9167e-11
24	99	1700	98.999999998071857	1.9476e-11	99.000000002403709	2.4280e-11

Table 2: Comparison of computed eigenvalues for Example 2 using the method of order 8 for sufficient values of N.

$\alpha = 3$			
i	N	λ_i	λ_i^*
0	300	3.4505626896	3.4505626899
24	1400	228.52088121	228.52088139
$\alpha = 4$			
0	300	3.7996730291	3.7996730298
24	800	397.14057994	397.14132678
$\alpha = 5$			
0	300	4.0891608366	4.0891593149
24	900	588.18981517	588.17824969

Table 3: Computed eigenvalues for Example 2, using the method of order 8 for several values of N.

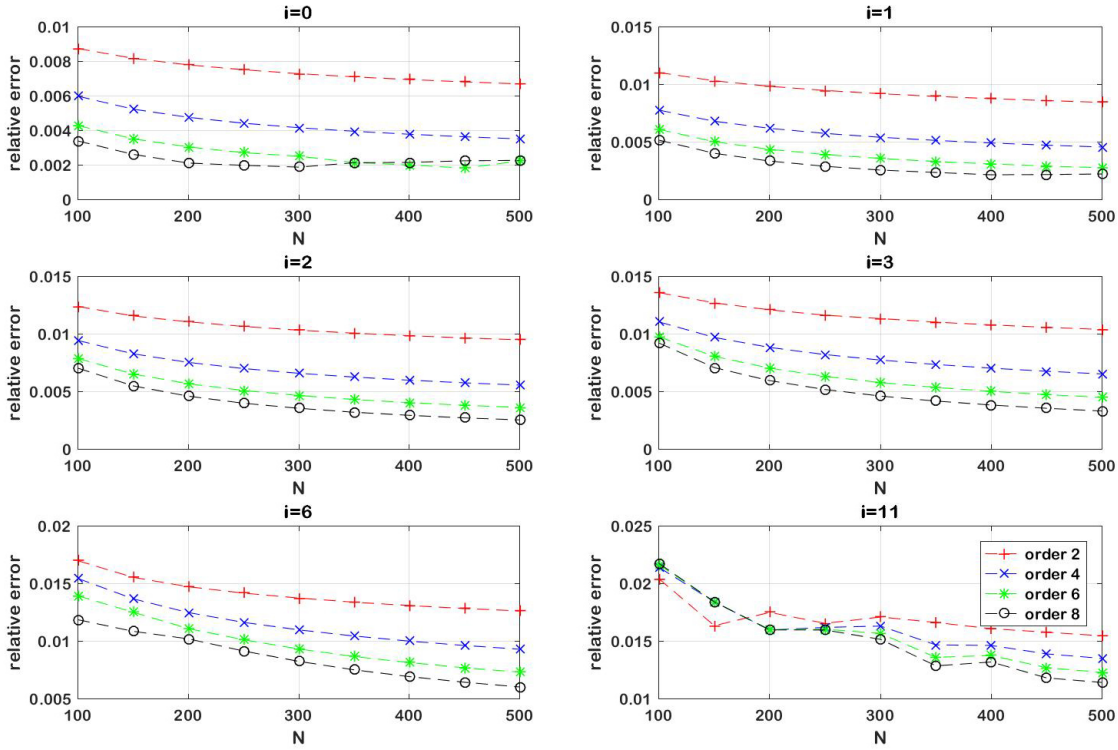

Figure 1: Relative errors in the computed eigenvalues for Example 3 versus N.

Example 3 In this example we focus on the Coulomb potential equation,

$$-y''(x) - \frac{1}{x}y(x) = \lambda y(x), \qquad x \in (0, \infty). \tag{36}$$

From [1] we know that the exact eigenvalues are

$$\lambda_i^* = -\frac{1}{4(i+1)^2}, \quad i \in \mathbb{N}. \tag{37}$$

Figure 1 shows the relative errors in the computed eigenvalues λ_0, λ_1, λ_2, λ_3, λ_6 and λ_{11} of the Coulomb potential problem versus N. The analysis of the results presented in Figure 1 confirms the results indicated in the previous examples: the approximate eigenvalues converge faster to the exact eigenvalues whenever the order of the method is greater. On the other hand, the use of a finer mesh is mandatory in order to have more accurate approximations of the greater eigenvalues.

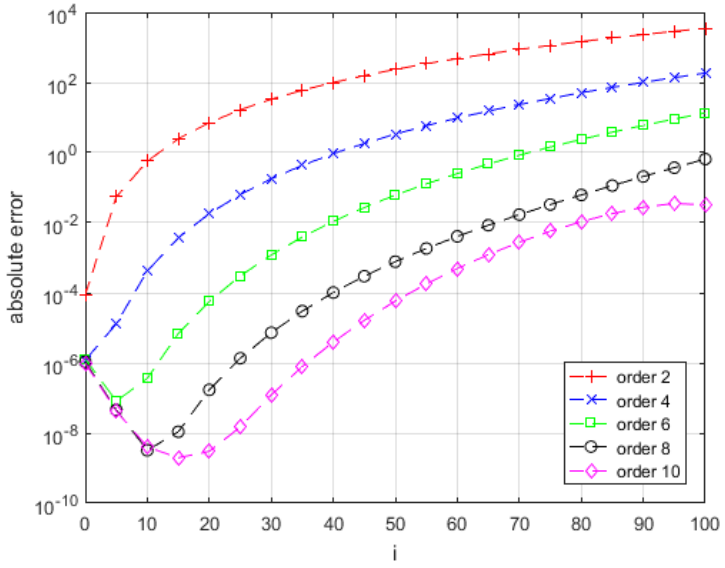

Figure 2: Absolute errors in the approximations of λ_i for Example 4 with $N = 500$.

Example 4 In this last example we consider the SLP (1) with

$$p(x) = \frac{\pi}{2\phi}((x\phi)^2 + 1), \quad q(x) = 1, \quad \omega(x) = \frac{1}{p(x)}.$$

By using the substitution given in (3) we obtain the following problem in Liouville normal form:

$$-z''(\tilde{x}) + \frac{\pi}{2\phi}\sec^2\left(\frac{\pi}{2}\tilde{x}\right) z(\tilde{x}) = \lambda z(\tilde{x}), \qquad z(0) = z(1) = 0.$$

Since the exact eigenvalues λ_i of this problem are not know in closed form, we consider as 'exact' the eigenvalues provided using the method of order 12 defined on the uniform mesh with $N = 2000$. In Figure 2 the errors in the eigenvalue estimates are reported. These results refer to methods of order $\rho = 2, 4, 6, 8, 10$ with $N = 500$. As one can see, the higher the order of the method the longer is the string of eigenvalues obtained with a certain accuracy. This is in perfect agreement with the result of Theorem 2, also in consideration of the fact that we have experimentally verified that the condition number of U is independent of N (e.g. $\text{cond}(U) \approx 5$ when $\rho = 4$).

5. Conclusions

In this paper we have proposed a technique to efficiently solve the Sturm-Liouville problems defined on semi-infinite intervals. This technique consists of a change of variable that transforms the problem defined on a semi-finite interval into one over a finite interval. Using finite difference schemes on the resulting problem we get an algebraic eigenvalue problem. The numerical results shown the effectiveness of the proposed approach.

It is worth to mention that this technique is also applicable to the standard boundary value problems for ordinary differential equations posed on semi-infinite interval.

The future of this research is concerned with the generalization of this approach in order to manage problems defined over an infinite interval.

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