INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 18, Number 1, Pages 62–78

WEAKLY REGULAR STURM-LIOUVILLE PROBLEMS: A CORRECTED SPECTRAL MATRIX METHOD

CECILIA MAGHERINI

Abstract. In this paper, we consider weakly regular Sturm-Liouville eigenproblems with unbounded potential at both endpoints of the domain. We propose a Galerkin spectral matrix method for its solution and we study the error in the eigenvalue approximations it provides. The result of the convergence analysis is then used to derive a low-cost and very effective formula for the computation of corrected numerical eigenvalues. Finally, we present and discuss the results of several numerical experiments which confirm the validity of the approach.

Key words. Sturm-Liouville eigenproblems, spectral matrix methods, Legendre polynomials, acceleration of convergence.

1. Introduction

Recently, the author studied a corrected spectral matrix method for solving weakly regular and singular Sturm-Liouville problems defined over the bounded domain $(-1,1)$ with an unbounded potential at the left endpoint, [13]. The numerical results provided by such technique are definitely satisfactory for weakly regular problems. This suggested to study a generalization of the method for the approximation of the eigenvalues and of the eigenfunctions of problems of the following type

$$-y''(x)+q(x)y(x) = \lambda y(x), \qquad x\in(-1,1)\,, \tag{1}$$

$$\alpha_L y(-1)+\beta_L y'(-1) = 0\,, \qquad \alpha_L^2+\beta_L^2\neq 0, \tag{2}$$

$$\alpha_R y(\,1)+\beta_R y'(\,1) = 0\,, \qquad \alpha_R^2+\beta_R^2\neq 0, \tag{3}$$

where the potential q is given by

$$q(x)=\sum_{i=1}^{S}\frac{g_i(x)}{(1-x)^{\beta_i}(1+x)^{\gamma_i}}, \qquad \beta_i,\gamma_i<1, \quad i=1,\ldots,S, \tag{4}$$

with functions g_i at the numerators that are analytical inside and on a Bernstein ellipse containing $[-1,1]$. In the literature, problems of this type with q unbounded at least at one endpoint are sometimes called weakly regular and it is well known that their spectrum is composed by real and simple eigenvalues which can be ordered as an increasing sequence tending to infinity. We will number them starting from index $k=1$, i.e. we will call

$$\{\lambda_1<\lambda_2<\lambda_3<\ldots\}$$

the exact spectrum of (1)–(4).

Before proceeding, it is to be said that Sturm-Liouville eigenproblems have many applications in physics, chemistry, biology, mechanics, and so on as described, for example, in [14, 20]. Their numerical solution has been studied extensively and many schemes/codes are available nowadays (see [1, 2, 3, 4, 5, 6, 8, 11, 12, 15, 16, 17, 18, 22, 23, 24] and references therein, to mention just a few).

Received by the editors July 2, 2020 and, in revised form, October 22, 2020.
2000 *Mathematics Subject Classification.* 65L15, 65L60, 65L70, 65B99.

Now, regarding problems with a potential function of the form specified in (4), in [13] we considered only the case $S = 2$ with $\beta_1 = \gamma_1 = \beta_2 = 0$, namely problems with a potential of the form $q(x) = g_1(x) + g_2(x)/(1+x)^{\gamma_2}$, and a special algorithm for $\gamma_2 \in (0, 1)$ and $y(-1) \neq 0$ was derived. As remarked in the same paper, the results obtained appear to be competitive with those given by other well-known schemes based on shooting techniques, [4, 11, 12, 15]. A possible explanation may be that we did not need to use a layer for handling the unbounded (but integrable) potential at the left endpoint. Concerning alternative matrix methods based on a spectral collocation approach, it must be said that a number of them, like the ones studied in [5, 8, 18, 24], refer to problems subject to the Dirichlet condition at both the endpoints.

These considerations justify the interest in generalizing the method proposed in [13] and the outline of this paper is the following. In Section 2, we recall the basic facts concerning the spectral Legendre-Galerkin matrix method introduced in [13] and we discuss the computation of the coefficient matrix that corresponds to a potential q of the form in (4). An analysis of the error in the numerical eigenvalues with respect to the generalized eigenvalue problem size is carried out in Section 3. In addition, in the same section, we derive a low cost and effective procedure for an a posteriori correction of the numerical eigenvalues. Finally, in Section 4 we report and discuss the results of some numerical experiments.

2. Spectral Legendre-Galerkin method

Let Π_{N+1} be the space of polynomials of maximum degree $N + 1$, for a fixed $N \in \mathbb{N}$, and let

$$\mathcal{S}_N \equiv \{r \in \Pi_{N+1} : \quad \alpha_L\, r(-1) + \beta_L\, r'(-1) = \alpha_R\, r(1) + \beta_R\, r'(1) = 0\} \tag{5}$$

$$\equiv \operatorname{span}(\mathcal{R}_0, \mathcal{R}_1, \ldots, \mathcal{R}_{N-1}). \tag{6}$$

We look for an approximation of an eigenfunction y of the following type

$$z_N(x) = \sum_{n=0}^{N-1} \zeta_{n,N} \mathcal{R}_n(x) \approx y(x) \tag{7}$$

where the coefficients $\zeta_{n,N}$ and the numerical eigenvalue $\lambda^{(N)}$ are determined by imposing, see (1),

$$\sum_{n=0}^{N-1} \left\langle \mathcal{R}_m, -\mathcal{R}_n'' + (q - \lambda^{(N)})\mathcal{R}_n \right\rangle \zeta_{n,N} = 0, \quad \text{for each } m = 0, \ldots, N-1. \tag{8}$$

Here $\langle \cdot, \cdot \rangle$ is the standard inner product in $L_2([-1, 1])$, i.e.

$$\langle u, v \rangle = \int_{-1}^{1} u(x)v(x)dx, \qquad u, v \in L_2([-1, 1]),$$

which is naturally suggested by the Liouville normal form of the SLP we are studying. We can write (8) as the following generalized eigenvalue problem

$$(A_N + Q_N)\, \boldsymbol{\zeta}_N = \lambda^{(N)} B_N \boldsymbol{\zeta}_N \tag{9}$$

where $\boldsymbol{\zeta}_N = (\zeta_{0N}, \ldots, \zeta_{N-1,N})^T$,

$$A_N = (a_{mn}), \quad B_N = (b_{mn}), \quad Q_N = (q_{mn}), \quad m, n = 0, \ldots, N-1, \tag{10}$$

with

$$a_{mn} = -\langle \mathcal{R}_m, \mathcal{R}_n'' \rangle, \quad b_{mn} = \langle \mathcal{R}_m, \mathcal{R}_n \rangle, \quad q_{mn} = \langle \mathcal{R}_m, q\, \mathcal{R}_n \rangle. \tag{11}$$

TABLE 1. Coefficients ξ_n, η_n and θ_n for some BCs.

BCs		ξ_n	η_n	θ_n
$y(\pm 1) = 0$	$n \geq 0$	1	0	-1
$y'(\pm 1) = 0$	$n \geq 0$	1	0	$-\frac{n(n+1)}{(n+2)(n+3)}$
$y(-1) = 0$ $y'(1) = 0$	$n \geq 0$	1	$\frac{(2n+3)}{(n+2)^2}$	$-\left(\frac{n+1}{n+2}\right)^2$
$y'(-1) = 0$ $y(1) = 0$	$n \geq 0$	1	$-\frac{(2n+3)}{(n+2)^2}$	$-\left(\frac{n+1}{n+2}\right)^2$
$y'(-1) = y(-1)$ $y'(1) = 0$	$n \geq 0$	1	$\frac{2(2n+3)}{(n+2)^2(2+(n+1)(n+3))}$	$-\frac{(n+1)^2(2+n(n+2))}{(n+2)^2(2+(n+1)(n+3))}$
$y'(\pm 1) = y(\pm 1)$	$n = 0$	$\frac{2}{3}$	1	$\frac{1}{3}$
	$n \geq 1$	1	$\frac{4(2n+3)}{(n+1)(n+2)^2(n+3)-4}$	$-\frac{n(n+1)^2(n+2)+4}{(n+1)(n+2)^2(n+3)-4}$

The matrices B_N and Q_N are clearly symmetric. The same property holds for A_N thanks to the well-known Green's identity by which one gets

$$a_{mn} - a_{nm} = \left[\mathcal{R}'_m(x)\mathcal{R}_n(x) - \mathcal{R}_m(x)\mathcal{R}'_n(x)\right]_{-1}^{1}.$$

Therefore if $\mathcal{R}_m$ and $\mathcal{R}_n$ belong to $\mathcal{S}_{\mathcal{N}}$ then it is possible to verify with some computations that $\mathcal{R}'_m(\pm 1)\mathcal{R}_n(\pm 1) - \mathcal{R}_m(\pm 1)\mathcal{R}'_n(\pm 1) = 0$ and consequently $a_{mn} = a_{nm}$.

The basis function $\mathcal{R}_n$ is chosen as follows [18]

$$\mathcal{R}_n(x) = \xi_n \mathcal{P}_n(x) + \eta_n \mathcal{P}_{n+1}(x) + \theta_n \mathcal{P}_{n+2}(x) \tag{12}$$

where $\mathcal{P}_j$ is the Legendre polynomial of degree j and the three coefficients ξ_n, η_n and θ_n are such that $\mathcal{R}_n$ verifies the boundary conditions (BCs), see (5)-(6). The complete discussion of the computation of such coefficients can be found in [13] where we used the fact that

$$\mathcal{P}_j(1) = (-1)^j \mathcal{P}_j(-1) = 1, \qquad \mathcal{P}'_j(1) = (-1)^{j-1}\mathcal{P}'_j(-1) = j(j+1)/2 \tag{13}$$

and we decided to use basis functions that verify $\|\mathcal{R}_n\|_\infty \leq 3$ for each $n \in \mathbb{N}_0$. This is obtained by imposing $\| (\xi_n, \eta_n, \theta_n)^T \|_\infty = 1$. Here we simply list in Table 1 the three coefficients of the linear combination in (12) for the four problems subject to natural BCs and for two general ones of Robin type.

Remark 2.1. *We shall proceed by assuming that $\xi_n \neq 0$ for each $n \in \mathbb{N}_0$. This ensures the validity of (5)-(6). Indeed, for rather particular BCs and for at most two values of n, one may need to replace $\mathcal{R}_n$ with a polynomial that belongs to $\mathcal{S}_N \cap span(\mathcal{P}_n, \mathcal{P}_{n+1}, \ldots, \mathcal{P}_{n+4})$ which is not orthogonal to $\mathcal{P}_n$ or quasi orthogonal to it. As previously said, in the sequel we shall assume that the BCs are such that it is not necessary to apply the described shrewdness.*

For later reference, it is important to underline the fact that, as soon as n is sufficiently large, we always got

$$\xi_n = 1, \tag{14}$$

$$\theta_n = -1 + O(n^{-1}), \tag{15}$$

$$\eta_n = \begin{cases} 0, & \text{if } \alpha_L\beta_R + \alpha_R\beta_L = 0, \\ O(n^{-1}) & \text{if } \alpha_L\beta_R + \alpha_R\beta_L \neq 0 \text{ and } \beta_L\beta_R = 0, \\ O(n^{-3}) & \text{if } \alpha_L\beta_R + \alpha_R\beta_L \neq 0 \text{ and } \beta_L\beta_R \neq 0. \end{cases} \tag{16}$$

More precisely, if the BCs are symmetric, i.e. if $\alpha_L\beta_R + \alpha_R\beta_L = 0$, then we always set $\eta_n = 0$ so that $\mathcal{R}_n$ is an even or an odd function if n is even or odd, respectively.

2.1. The matrices A_N and B_N. In this section, we recall the results obtained in [13] about the entries of A_N and B_N in (10)-(11).
Concerning the first matrix, one immediately gets that $a_{mn} = 0$ for each $m > n$ since $\mathcal{R}_m$ is orthogonal to any polynomial in Π_{m-1}, see (12). Consequently, $A_N = A_N^T$ is diagonal with diagonal entries

$$\begin{aligned} a_{nn} &= -\xi_n\theta_n\langle \mathcal{P}_n, \mathcal{P}''_{n+2}\rangle \\ &= -\xi_n\theta_n \left[\mathcal{P}_n(x)\mathcal{P}'_{n+2}(x) - \mathcal{P}'_n(x)\mathcal{P}_{n+2}(x)\right]_{-1}^{1} \\ &= -2(2n+3)\xi_n\theta_n, \end{aligned} \tag{17}$$

see (13). We remark that, independently of the BCs, a_{nn} satisfies

$$a_{nn} = 4\left(n + \frac{3}{2}\right)\left(1 + O\left(n^{-1}\right)\right), \quad n \gg 1. \tag{18}$$

Regarding B_N, it is not too difficult to verify that it is pentadiagonal. In more detail, if we let

$$\hat{b}_n = \langle \mathcal{P}_n, \mathcal{P}_n\rangle = 2/(2n+1),$$

$$\hat{B}_N = \begin{pmatrix} \hat{b}_0 & & \\ & \ddots & \\ & & \hat{b}_{N+1} \end{pmatrix}, \quad R_N = \begin{pmatrix} \xi_0 & & & \\ \eta_0 & \ddots & & \\ \theta_0 & \ddots & \ddots & \\ & \ddots & \ddots & \xi_{N-1} \\ & & \ddots & \eta_{N-1} \\ & & & \theta_{N-1} \end{pmatrix}, \tag{19}$$

then we get

$$B_N = R_N^T\,\hat{B}_N R_N. \tag{20}$$

2.2. The matrix Q_N. From (10)-(11), one obtains that Q_N admits a factorization similar to the one just given for B_N. Specifically

$$Q_N = R_N^T\,\hat{Q}_N R_N, \qquad \hat{Q}_N = (\hat{q}_{mn}) \tag{21}$$

where R_N is defined in (19),

$$\hat{q}_{mn} = \langle \mathcal{P}_m, q\mathcal{P}_n\rangle = \sum_{i=1}^{S}\langle \mathcal{P}_m, g_i\mathcal{P}_n\rangle_{(\beta_i,\gamma_i)} \equiv \sum_{i=1}^{S}\hat{q}_{mn}^{(i)}, \tag{22}$$

being

$$\langle u, v\rangle_{(\beta,\gamma)} = \int_{-1}^{1}\frac{u(x)\,v(x)}{(1-x)^{\beta}\,(1+x)^{\gamma}}dx, \qquad \beta, \gamma < 1. \tag{23}$$

As done in [10, 13], it is possible to prove the following result by using the well-known recurrence relation of the Legendre polynomials.

Proposition 2.1. *Let $q \in L_1((-1,1))$ and*

$$\hat{\mathbf{q}}_n \equiv (\hat{q}_{0n}, \hat{q}_{1n}, \ldots)^T \in \ell_\infty, \quad n \geq 0.$$

If we define the linear tridiagonal operator $\mathbf{z} \in \ell_\infty \mapsto \mathcal{H}\,\mathbf{z} \in \ell_\infty$ where

$$\mathcal{H} = \begin{pmatrix} 0 & h_{01} & & & \\ h_{10} & 0 & h_{12} & & \\ & h_{21} & 0 & h_{23} & \\ & & \ddots & \ddots & \ddots \end{pmatrix}, \qquad \begin{aligned} h_{m,m-1} &= m/(2m+1), \\ h_{m,m+1} &= (m+1)/(2m+1), \end{aligned}$$

and we let $\hat{\mathbf{q}}_{-1}$ be the zero sequence, then we get

$$\hat{\mathbf{q}}_{n+1} = \frac{2n+1}{n+1}\,\mathcal{H}\hat{\mathbf{q}}_n - \frac{n}{n+1}\,\hat{\mathbf{q}}_{n-1}, \qquad n \geq 0. \qquad \square \tag{24}$$

Now, the structure of $\mathcal{H}$ and (24) permit to determine the entire matrix $\hat{Q}_N$ once $\hat{q}_{m0}$ have been computed for each $m = 0, 1, \ldots, 2N+2$ (see [10, 13] for the details). We shall proceed by discussing how we determine these values for problems with $S = 1$ since the generalization is simple, see (22). In this regard, we observe that (23), [9, 16.4 formula (2)] and arguments similar to the ones used in the proof of [10, Proposition 2] allow to get that

$$\hat{\mathbf{q}}_0 = g_1(\mathcal{H}) \begin{pmatrix} \hat{q}_0^{(1)} \\ \hat{q}_1^{(1)} \\ \vdots \end{pmatrix}, \quad \hat{q}_m^{(1)} = \langle \mathcal{P}_m, \mathcal{P}_0 \rangle_{(\beta_1,\gamma_1)} = \langle \mathcal{P}_m, 1 \rangle_{(\beta_1,\gamma_1)}, \tag{25}$$

where, recalling that g_1 is analytical inside and over a Bernstein ellipse containing $[-1,1]$ by assumption, the operator $g_1(\mathcal{H})$ is defined as $g_1(\mathcal{H}) = \sum_{\ell=0}^{+\infty} \frac{\langle g_1, \mathcal{P}_\ell \rangle}{\langle \mathcal{P}_\ell, \mathcal{P}_\ell \rangle}\, \mathcal{P}_\ell(\mathcal{H})$.

Now, let us suppose for the moment that we have computed the values of $\hat{q}_m^{(1)}$ for each $m = 0, \ldots, L$ with L sufficiently large. Then, for the effective computation of the required entries of $\hat{\mathbf{q}}_0$ we proceed in this way. We get a polynomial approximation of g_1 by transforming it in a `Chebfun` function [7], which is accurate up to machine precision, and then we apply (25) to compute the first $2N+2$ entries of $\hat{\mathbf{q}}_0$.

Concerning the computation of $\hat{q}_m^{(1)}$ we have to distinguish the following cases:

(1) $\beta_1 = \gamma_1 = 0$: it is evident that $\hat{q}_0^{(1)} = 2$ and $\hat{q}_m^{(1)} = 0$ for each $m > 0$;
(2) $\beta_1 = 0, \gamma_1 \neq 0$: as discussed in [13] it results

$$\hat{q}_m^{(1)} = \frac{(-1)^m\, 2^{1-\gamma_1}\, (\gamma_1)_m}{(1-\gamma_1)_{m+1}} \tag{26}$$

where $(t)_\ell$ is the Pochhammer symbol;
(3) $\beta_1 \neq 0, \gamma_1 = 0$: with similar computations one gets

$$\hat{q}_m^{(1)} = \frac{2^{1-\beta_1}\, (\beta_1)_m}{(1-\beta_1)_{m+1}}; \tag{27}$$

(4) $\beta_1 \gamma_1 \neq 0$: by using [9, 16.2, formula(6)] we get

$$\hat{q}_m^{(1)} = \alpha\, {}_3F_2\left(\begin{matrix} -m,\ 1+m,\ 1-\beta_1 \\ 1,\ 2-\beta_1-\gamma_1 \end{matrix} ; 1 \right) \tag{28}$$

where

$$\alpha = \frac{2^{1-\beta_1-\gamma_1}\Gamma(1-\beta_1)\Gamma(1-\gamma_1)}{\Gamma(2-\beta_1-\gamma_1)} = \hat{q}_0^{(1)}. \tag{29}$$

It is clear that the formulas in (26) or (27) allow to compute $\hat{q}_m^{(1)}$ easily. For example, if $\beta_1 \neq 0$ and $\gamma_1 = 0$ then from (27) one gets

$$\hat{q}_0^{(1)} = \frac{2^{1-\beta_1}}{1-\beta_1}, \qquad \hat{q}_{m+1}^{(1)} = \frac{m+\beta_1}{m+2-\beta_1}\hat{q}_m^{(1)}, \quad m \geq 0,$$

so that it is possible to proceed recursively. On the other hand, if $\beta_1\gamma_1 \neq 0$ then the computation of the Gauss hypergeometric function at the right hand-side of (28) can be costly and ill-conditioned. We thus preferred to find alternative expressions. In particular, if $\beta_1 = \gamma_1 \neq 0$ then the application of the following Whipple sum

$${}_3F_2\left(\begin{array}{c} a,\ 1-a,\ c \\ e,\ 1+2c-e \end{array};1\right) = \frac{2^{1-2c}\pi\Gamma(e)\Gamma(1+2c-e)}{\Gamma((a+e)/2)\Gamma((a+1+2c-e)/2)\Gamma((e+1-a)/2)\Gamma((2+2c-a-e)/2)}$$

with $a = -m$, $c = 1-\gamma_1$ and $e = 1$ gives

$$\hat{q}_m^{(1)} = \frac{\pi\Gamma^2(1-\gamma_1)}{\Gamma\left((3-2\gamma_1+m)/2\right)\Gamma\left((2-2\gamma_1-m)/2\right)\Gamma\left((2+m)/2\right)\Gamma\left((1-m)/2\right)}.$$

Therefore, if m is odd then $\hat{q}_m^{(1)} = 0$ (this was indeed already evident from its definition in (25) with $\beta_1 = \gamma_1$). On the other hand, if m is even then

$$\begin{aligned} \hat{q}_0^{(1)} &= \frac{\sqrt{\pi}\,\Gamma(1-\gamma_1)}{\Gamma(3/2-\gamma_1)} = \frac{2^{1-2\gamma_1}\,\Gamma^2(1-\gamma_1)}{\Gamma(2-2\gamma_1)}, \\ \hat{q}_{m+2}^{(1)} &= \frac{(m+2\gamma_1)(m+1)}{(m+3-2\gamma_1)(m+2)}\,\hat{q}_m^{(1)}, \qquad m = 0,2,4,\ldots. \end{aligned}$$

Remark 2.2. *If $q(x) = q(-x)$ and N is even then the matrix $\hat{Q}_N$ in (21) is permutation similar to a 2×2 block diagonal matrix with diagonal blocks of size $N/2+1$. In addition, if the coefficients of the BCs in (2)-(3) verify $\alpha_L\beta_R + \alpha_R\beta_R = 0$ then the SLP is called symmetric and, as we recalled after (16), $\eta_n = 0$ for each n. Therefore, the matrices A_N, Q_N and B_N are permutation similar to 2×2 block diagonal matrices too, see the paragraph before (17) and (19)–(21). This implies that we can split the generalized eigenvalue problem (9) into two ones of halved size.*

It remains to discuss how it is possible to avoid the evaluation of the Gauss hypergeometric function for the computation of $\hat{q}_m^{(1)}$ if $\beta_1\gamma_1 \neq 0$ and $\beta_1 \neq \gamma_1$. In this case, even though alternative strategies are possible, we decided to write $\mathcal{P}_m \equiv \mathcal{P}_m^{(0,0)}$ as a linear combination of $\left\{\mathcal{P}_\ell^{(0,-\gamma_1)}\right\}_{\ell=0}^{m}$ where $\mathcal{P}_\ell^{(0,-\gamma_1)}$ is the Jacobi polynomial of degree ℓ with weighting function $\omega(x) = (1+x)^{-\gamma_1}$. In other words, first of all we write

$$\mathcal{P}_m(x) \equiv \mathcal{P}_m^{(0,0)}(x) = \sum_{\ell=0}^{m} \chi_{m,\ell}\mathcal{P}_\ell^{(0,-\gamma_1)}(x).$$

Then we determine $\hat{q}_m^{(1)}$ as follows

$$\hat{q}_m^{(1)} = \sum_{\ell=0}^{m} \chi_{m,\ell}\,\langle \mathcal{P}_\ell^{(0,-\gamma_1)}, 1\rangle_{(\beta_1,\gamma_1)}.$$

Now, by using formulas in [9, 16.4] we obtain

$$\begin{aligned}\chi_{m,\ell} &= \frac{\langle \mathcal{P}_m^{(0,0)}, \mathcal{P}_\ell^{(0,-\gamma_1)}\rangle_{(0,\gamma_1)}}{\langle \mathcal{P}_\ell^{(0,-\gamma_1)}, \mathcal{P}_\ell^{(0,-\gamma_1)}\rangle_{(0,\gamma_1)}} \\ &= \frac{\Gamma(1-\gamma_1)(2\ell+1-\gamma_1)\Gamma(m+\ell+1)\Gamma(\ell+1-\gamma_1)}{\Gamma(\ell+1)\,\Gamma(m+\ell+2-\gamma_1)\Gamma(m-\ell+1)\Gamma(\ell-m+1-\gamma_1)}, \\ \langle \mathcal{P}_\ell^{(0,-\gamma_1)}, 1\rangle_{(\beta_1,\gamma_1)} &= \frac{2^{1-\beta_1-\gamma_1}\Gamma(1-\beta_1)\Gamma(\ell+1-\gamma_1)(\beta_1)_\ell}{\Gamma(2-\beta_1-\gamma_1)\,\Gamma(\ell+1)\,(2-\beta_1-\gamma_1)_\ell}.\end{aligned}$$

Hence

$$\hat{q}_m^{(1)} = \alpha \sum_{\ell=0}^{m} t_{m-\ell} u_{m+\ell} \nu_\ell,$$

where α is defined in (29),

$$\begin{aligned} t_r &= \frac{1}{\Gamma(1+r)\Gamma(1-\gamma_1-r)}, \qquad u_r = \frac{\Gamma(r+1)}{\Gamma(r+2-\gamma_1)}, \\ \nu_\ell &= (2\ell+1-\gamma_1)\left(\frac{\Gamma(\ell+1-\gamma_1)}{\Gamma(\ell+1)}\right)^2 \frac{(\beta_1)_\ell}{(2-\beta_1-\gamma_1)_\ell}. \end{aligned}$$

It is not too difficult to verify that

$$\begin{pmatrix} \hat{q}_0^{(1)} \\ \hat{q}_1^{(1)} \\ \hat{q}_2^{(1)} \\ \hat{q}_3^{(1)} \\ \vdots \end{pmatrix} = \alpha\,(T \circ U) \begin{pmatrix} \nu_0 \\ \nu_1 \\ \nu_2 \\ \nu_3 \\ \vdots \end{pmatrix}, \tag{30}$$

being "$\circ$" the Hadamard product and

$$T = \begin{pmatrix} t_0 & & & & \\ t_1 & t_0 & & & \\ t_2 & t_1 & t_0 & & \\ t_3 & t_2 & t_1 & t_0 & \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}, \qquad U = \begin{pmatrix} u_0 & u_1 & u_2 & u_3 & \dots \\ u_1 & u_2 & u_3 & & \\ u_2 & u_3 & & & \\ u_3 & & & & \\ \vdots & & & & \end{pmatrix},$$

i.e. T and U are a lower triangular Toeplitz and an Hankel matrix, respectively. Clearly, a suitable truncation of the vectors and matrices in (30) is operated depending on the number of values of $\hat{q}_m^{(1)}$ that we actually need. In addition, we compute ν_ℓ, t_r and u_r recursively. Finally, it is worth mentioning that an algorithm similar to the one described in [21] can be used for the matrix-vector product in (30).

2.3. Computational cost. The main steps which contribute to the computational cost of the proposed method are the computation of the matrix $\hat{Q}_N$ in (21)-(22) and the solution of the generalized eigenvalue problem in (9). In fact, from (17)–(21) one deduces that the other terms, namely the costs for getting A_N and B_N and the computation of Q_N once $\hat{Q}_N$ has been determined, are surely negliglible with respect to the former ones.

Concerning the matrix $\hat{Q}_N$ the described technique requires the computation of S `Chebfun` functions, for the g_i functions at the numerators in (4), and the application of (24)-(25) which require, at most and depending on the value of the couples (β_i, γ_i), a number of floating-point operations proportional to $S\,N^2$ (see

also (30)).
Regarding the solution of (9), it is to be remarked that routines of numerical linear algebra which take advantage of the facts that $A_N + Q_N$ is symmetric and B_N is symmetric positive definite can be conveniently employed.

3. Error analysis and computation of corrected numerical eigenvalues

We now study the behavior of the error in the resulting numerical eigenvalues as N increases and for a fixed index. In particular, we consider weakly regular problems with a potential of the type specified in (4) which is unbounded at least at one endpoint. The analysis that we are going to present will be also used to derive a very effective and efficient procedure for an a posteriori correction of the numerical eigenvalues.

Let $\lambda^{(N)}$ be the approximation of the exact eigenvalue λ as N increases[1] and let y be the corresponding exact eigenfunction having the following expansion

$$y(x) = \sum_{n=0}^{+\infty} c_n \mathcal{R}_n(x). \tag{31}$$

The following first result can be proved by using arguments similar to the ones considered in [13].

Theorem 3.1. *If N is sufficiently larger than the index of the eigenvalue then, see (7) and (17),*

$$\begin{aligned} c_n &\approx -\frac{\langle \mathcal{R}_n, qy\rangle}{a_{nn}} = -\sum_{i=1}^{S} \frac{\langle \mathcal{R}_n, g_i y\rangle_{(\beta_i,\gamma_i)}}{a_{nn}}, \\ \lambda - \lambda^{(N)} &\approx -\frac{1}{\langle z_N, y\rangle} \sum_{n=N}^{+\infty} c_n \langle \mathcal{R}_n, qz_N\rangle \approx -\frac{1}{\langle z_N, y\rangle} \sum_{i,j=1}^{S} \Delta_{ij} \end{aligned} \tag{32}$$

where

$$\Delta_{ij} = \sum_{n=N}^{+\infty} \frac{1}{a_{nn}} \langle \mathcal{R}_n, g_i y\rangle_{(\beta_i,\gamma_i)} \langle \mathcal{R}_n, g_j z_N\rangle_{(\beta_j,\gamma_j)}. \quad \square \tag{33}$$

The asymptotic estimate that we are going to prove in the next theorem is fundamental for proceeding.

Theorem 3.2. *Let $\psi \in C^\infty(-1,1) \bigcap C^1[-1,1]$. If $\psi(-1)\,\psi(1) \neq 0$, $\beta, \gamma < 1$ and if n is sufficiently large then*

$$\langle \mathcal{R}_n, \psi\rangle_{(\beta,\gamma)} \approx \frac{(-1)^n 2\,\omega(-1,\gamma,\beta)\,\psi(-1)}{(n+3/2)^{p(\gamma)/2}} + \frac{2\,\omega(+1,\beta,\gamma)\,\psi(1)}{(n+3/2)^{p(\beta)/2}}, \tag{34}$$

where

$$p(\delta) = 6 - 4\delta, \qquad \omega(\pm 1, \delta_0, \delta_1) = 2(2 - \delta_0 - \kappa_{\pm 1})\,\hat{\omega}(\delta_0, \delta_1), \tag{35}$$

being

$$\kappa_{\pm 1} = \begin{cases} 1, & \text{if } \mathcal{R}_n(\pm 1) = 0 \\ 0, & \text{otherwise} \end{cases}, \quad \hat{\omega}(\delta_0, \delta_1) = \frac{2^{1-\delta_0-\delta_1}\Gamma(1-\delta_0)}{\Gamma(\delta_0)}. \tag{36}$$

[1] As usual when working with matrix methods, if λ is the eigenvalue of index k then $\lambda^{(N)}$ is the kth smallest eigenvalue of the generalized eigenvalue problem.

Proof. Recalling the definition of $\mathcal{R}_n$ in (12), let us consider first of all $\langle \mathcal{P}_n, \psi \rangle_{(\beta,\gamma)}$. In this regard, if we use the results proved in [19], (25)–(27) and we assume that n is sufficiently large then we get

$$\begin{aligned}
\langle \mathcal{P}_n, \psi \rangle_{(\beta,\gamma)} &\approx \frac{\psi(-1)}{2^\beta} \langle \mathcal{P}_n, 1 \rangle_{(0,\gamma)} + \frac{\psi(1)}{2^\gamma} \langle \mathcal{P}_n, 1 \rangle_{(\beta,0)} \\
&= \frac{\psi(-1)\,(-1)^n\,(\gamma)_n}{2^{\beta+\gamma-1}(1-\gamma)_{n+1}} + \frac{\psi(1)\,(\beta)_n}{2^{\beta+\gamma-1}(1-\beta)_{n+1}} \\
&= \frac{\psi(-1)\,(-1)^n\,\hat{\omega}(\gamma,\beta)\,\Gamma(n+\gamma)}{\Gamma(n+2-\gamma)} + \frac{\psi(1)\,\hat{\omega}(\beta,\gamma)\,\Gamma(n+\beta)}{\Gamma(n+2-\beta)}.
\end{aligned}$$

Now, it is known that the ratio of two gamma functions satisfies

$$\frac{\Gamma(z+a)}{\Gamma(z+b)} = z^{a-b}\left(1 + \frac{(a-b)(a+b-1)}{2z} + O(z^{-2})\right), \quad z \gg 0.$$

Therefore, if we use it with $z = n + 1/2$ then we obtain

$$\langle \mathcal{P}_n, \psi \rangle_{(\beta,\gamma)} \approx \left(\frac{\psi(-1)\,(-1)^n\,\hat{\omega}(\gamma,\beta)}{(n+1/2)^{\hat{p}(\gamma)}} + \frac{\psi(1)\,\hat{\omega}(\beta,\gamma)}{(n+1/2)^{\hat{p}(\beta)}}\right)\left(1 + O(n^{-2})\right),$$

with

$$\hat{p}(\delta) = 2 - 2\delta = \frac{p(\delta)}{2} - 1, \qquad \delta = \gamma, \beta. \tag{37}$$

This implies that to determine an estimate for $\langle \mathcal{R}_n, \psi \rangle_{(\beta,\gamma)}$, we have to study these terms

$$\begin{aligned}
&(-1)^n\left(\frac{\xi_n}{(n+1/2)^{\hat{p}(\gamma)}} - \frac{\eta_n}{(n+3/2)^{\hat{p}(\gamma)}} + \frac{\theta_n}{(n+5/2)^{\hat{p}(\gamma)}}\right) \\
&\qquad \approx (-1)^n\left(n+\frac{3}{2}\right)^{-\hat{p}(\gamma)}\left(\xi_n - \eta_n + \theta_n + \frac{\hat{p}(\gamma)(\xi_n - \theta_n)}{n+3/2}\right), \\
&\frac{\xi_n}{(n+1/2)^{\hat{p}(\beta)}} + \frac{\eta_n}{(n+3/2)^{\hat{p}(\beta)}} + \frac{\theta_n}{(n+5/2)^{\hat{p}(\beta)}} \\
&\qquad \approx \left(n+\frac{3}{2}\right)^{-\hat{p}(\beta)}\left(\xi_n + \eta_n + \theta_n + \frac{\hat{p}(\beta)(\xi_n - \theta_n)}{n+3/2}\right).
\end{aligned}$$

We recall that if n is sufficiently large then $\xi_n = 1$, see (14). In addition, by using the formulas in [13], see also (15)-(16), it is possible to verify with some computations that

(1) if $\mathcal{R}_n(-1) = (-1)^n(\xi_n - \eta_n + \theta_n) \neq 0$ then

$$\xi_n - \eta_n + \theta_n = \frac{4}{n+3/2}\left(1 + O\left(\frac{1}{n}\right)\right);$$

(2) if $\mathcal{R}_n(1) = \xi_n + \eta_n + \theta_n \neq 0$ then

$$\xi_n + \eta_n + \theta_n = \frac{4}{n+3/2}\left(1 + O\left(\frac{1}{n}\right)\right);$$

(3) $\xi_n - \theta_n = 2\left(1 + O\left(n^{-1}\right)\right)$.

Therefore, see (36) and (37),

$$\begin{aligned}
\xi_n - \eta_n + \theta_n + \frac{\hat{p}(\gamma)(\xi_n - \theta_n)}{n+3/2} &\approx \frac{4(2-\gamma-\kappa_{-1})}{n+3/2} \\
\xi_n + \eta_n + \theta_n + \frac{\hat{p}(\beta)(\xi_n - \theta_n)}{n+3/2} &\approx \frac{4(2-\beta-\kappa_{+1})}{n+3/2}.
\end{aligned}$$

The statement follows by collecting all these partial results. □

It must be underlined that $\hat{\omega}(\delta_0, \delta_1) = 0$ if $-\delta_0 \in \mathbb{N}_0$, see (36). This implies that one or both the terms at the right hand-side of (34) can be zero. For our purposes, this does not constitute a problem since in the convergence analysis that we are going to prove such terms are surely negligible with respect to the others.

We need the following notation to proceed: for each $i = 1, \dots, S$, let

$$g_i(x) = (1-x)^{r_i}(1+x)^{\ell_i}\hat{g}_i(x), \quad \hat{g}_i(\pm 1) \neq 0, \tag{38}$$

i.e. let r_i and ℓ_i be the multiplicities of $x = 1$ and $x = -1$, as zeros of g_i, respectively. We are now ready for proving the following theorem.

Theorem 3.3 (Convergence)**.** *Let assume the potential in (4) is unbounded at least at one endpoint and let consider the following subsets of* $\{1, 2, \dots, S\}$

$$\begin{array}{rcll} \mathcal{I}_L & \subseteq & \{1,2,\dots,S\} & \text{with} \quad i \in \mathcal{I}_L \quad \longleftrightarrow \quad -\gamma_i \notin \mathbb{N}_0, \\ \mathcal{I}_R & \subseteq & \{1,2,\dots,S\} & \text{with} \quad i \in \mathcal{I}_R \quad \longleftrightarrow \quad -\beta_i \notin \mathbb{N}_0. \end{array}$$

If N is sufficiently larger than the index of the eigenvalue then

$$\lambda - \lambda^{(N)} = O\left((N+1)^{-p}\right), \qquad p = \inf\left(p_L, p_R\right), \tag{39}$$

where, see (35)-(36) and (38),

$$\begin{array}{rcll} p_L & = & \inf\limits_{i \in \mathcal{I}_L} p(\hat{\gamma}_i) = \inf\limits_{i \in \mathcal{I}_L} 6 - 4\hat{\gamma}_i, & \hat{\gamma}_i = \gamma_i - \ell_i - \kappa_-, \\ p_R & = & \inf\limits_{i \in \mathcal{I}_R} p(\hat{\beta}_i) = \inf\limits_{i \in \mathcal{I}_R} 6 - 4\hat{\beta}_i, & \hat{\beta}_i = \beta_i - r_i - \kappa_+, \end{array}$$

being $\inf \emptyset = +\infty$ *by convention.*

Proof. From the definition of $\kappa_\pm$, (7) and (31) we get

$$y(x) = (1-x)^{\kappa_+}(1+x)^{\kappa_-}\hat{y}(x), \qquad \hat{y}(\pm 1) \neq 0, \tag{40}$$

$$z_N(x) = (1-x)^{\kappa_+}(1+x)^{\kappa_-}\hat{z}_N(x), \qquad \hat{z}_N(\pm 1) \neq 0, \tag{41}$$

so that recalling (32)-(33) we must determine an estimate for

$$\frac{1}{a_{nn}}\left(\langle \mathcal{R}_n, \hat{g}_i\hat{y}\rangle_{(\hat{\beta}_i,\hat{\gamma}_i)} \langle \mathcal{R}_n, \hat{g}_j\hat{z}_N\rangle_{(\hat{\beta}_j,\hat{\gamma}_j)}\right) \equiv (\star).$$

To this end, we apply (34) with $(\beta, \gamma) = (\hat{\beta}_i, \hat{\gamma}_i)$ and $\psi = \hat{g}_i\hat{y}$, or with $(\beta, \gamma) = (\hat{\beta}_j, \hat{\gamma}_j)$ and $\psi = \hat{g}_j\hat{z}_N$. In this way, recalling also (18), we obtain

$$\begin{aligned} (\star) \quad \approx \quad & \left(\frac{(-1)^n \sigma_{iL}\, \hat{y}(-1)}{(n+3/2)^{1+p(\hat{\gamma}_i)/2}} + \frac{\sigma_{iR}\, \hat{y}(1)}{(n+3/2)^{1+p(\hat{\beta}_i)/2}}\right) \\ & \times \left(\frac{(-1)^n \sigma_{jL}\, \hat{z}_N(-1)}{(n+3/2)^{p(\hat{\gamma}_j)/2}} + \frac{\sigma_{jR}\, \hat{z}_N(1)}{(n+3/2)^{p(\hat{\beta}_j)/2}}\right), \end{aligned}$$

where

$$\sigma_{iL} = \hat{g}_i(-1)\omega(-1, \hat{\gamma}_i, \hat{\beta}_i), \qquad \sigma_{iR} = \hat{g}_i(+1)\omega(+1, \hat{\beta}_i, \hat{\gamma}_i).$$

We now use the following integral estimates with suitable $\bar{p} > 0$:

$$\begin{aligned}
\sum_{n=N}^{+\infty} \frac{1}{(n+3/2)^{1+\bar{p}}} \quad &\approx \quad \int_N^{+\infty} (n+1)^{-1-\bar{p}} dn = \frac{1}{\bar{p}(N+1)^{\bar{p}}}, \\
& \quad \ell = \mathrm{rem}(N,2) \\
\sum_{n=N}^{+\infty} \frac{(-1)^n}{(n+3/2)^{1+\bar{p}}} \quad &\uparrow \\
&\approx \quad (-1)^N \sum_{m=(N-\ell)/2}^{+\infty} \frac{1+\bar{p}}{(2m+\ell+3/2)^{2+\bar{p}}} \\
&\approx \quad (-1)^N \int_{(N-\ell)/2}^{+\infty} \frac{(1+\bar{p})\ dm}{(2m+\ell+1)^{2+\bar{p}}} \\
&= \quad \frac{(-1)^N}{2(N+1)^{1+\bar{p}}}.
\end{aligned}$$

In particular, we apply the first one with $\bar{p} = (p(\hat{\gamma}_i) + p(\hat{\gamma}_j))/2$ or $\bar{p} = (p(\hat{\beta}_i) + p(\hat{\beta}_j))/2$ and the second estimate with $\bar{p} = (p(\hat{\gamma}_i) + p(\hat{\beta}_j))/2$ or with $\bar{p} = (p(\hat{\beta}_i) + p(\hat{\gamma}_j))/2$. This leads to, see (33),

$$\begin{aligned}
\Delta_{ij} \approx \bar{\Delta}_{ij} = \quad & \frac{2\,\sigma_{iL}\,\sigma_{jL}\hat{y}(-1)\hat{z}_N(-1)}{(p(\hat{\gamma}_i)+p(\hat{\gamma}_j))(N+1)^{(p(\hat{\gamma}_i)+p(\hat{\gamma}_j))/2}} \\
+ \quad & \frac{2\,\sigma_{iR}\,\sigma_{jR}\,\hat{y}(1)\hat{z}_N(1)}{(p(\hat{\beta}_i)+p(\hat{\beta}_j))(N+1)^{(p(\hat{\beta}_i)+p(\hat{\beta}_j))/2}} \\
+ \quad & \frac{(-1)^N\,\sigma_{iL}\,\sigma_{jR}\,\hat{y}(-1)\hat{z}_N(1)}{2(N+1)^{1+(p(\hat{\gamma}_i)+p(\hat{\beta}_j))/2}} \\
+ \quad & \frac{(-1)^N\,\sigma_{iR}\,\sigma_{jL}\,\hat{y}(1)\hat{z}_N(-1)}{2(N+1)^{1+(p(\hat{\beta}_i)+p(\hat{\gamma}_j))/2}}.
\end{aligned} \tag{42}$$

Therefore

$$\lambda - \lambda^{(N)} \approx -\frac{1}{\langle z_N, y\rangle} \sum_{i,j=1}^{S} \bar{\Delta}_{ij} \tag{43}$$

and the statement follows by observing that the principal term of such summation behaves like $O\left((N+1)^{-p}\right)$ where p is defined in (39). □

As done in [13], we now discuss how we can use (43) to improve the accuracy of the numerical eigenvalues. The approach is that of considering the following normalization for the numerical and the exact eigenfunctions, see (40)-(41),

$$\langle z_N, z_N\rangle = \boldsymbol{\zeta}_N^T B_N \boldsymbol{\zeta}_N = 1, \qquad \langle y, y\rangle = 1, \qquad \hat{z}_N(-1), \hat{y}(-1) > 0.$$

By using the orthogonality of the Legendre polynomials, the estimates $\langle z_N, y\rangle \approx 1$ and $\hat{y}(\pm 1) \approx \hat{z}_N(\pm 1)$ follow and consequently the next formula for the computation of corrected numerical eigenvalues

$$\mu^{(N)} = \lambda^{(N)} - \sum_{i,j=1}^{S} \hat{\Delta}_{ij} \tag{44}$$

where $\hat{\Delta}_{ij}$ is obtained from $\bar{\Delta}_{ij}$ via the substitutions $\hat{y}(\pm 1) \to \hat{z}_N(\pm 1)$, see (40)–(42). These are done by using $z_N(\pm 1)$ or $z'_N(\pm 1)$. For example, if $y(-1) = 0$ and $y(1) \neq 0$ then $y(x) = (1+x)\hat{y}(x)$ and $z_N(x) = (1+x)\hat{z}_N(x)$. Consequently

$$\hat{y}(1) = y(1)/2 \approx z_N(1)/2 = \hat{z}_N(1), \qquad \hat{y}(-1) = y'(-1) \approx z'_N(-1) = \hat{z}'_N(-1).$$

TABLE 2. Order of convergence for problems with potential (45).

$y'(-1) = y(1) = 0, \qquad p = p_L = 6 - 4 \times (1/4) = 5$						
N	$\delta\lambda_{5,N}$	order	$\delta\lambda_{10,N}$	order	$\delta\lambda_{20,N}$	order
49	4.4416E − 06	5.002	5.5319E − 06	4.993	4.8732E − 06	4.969
99	1.3859E − 07	5.001	1.7368E − 07	4.999	1.5556E − 07	4.996
199	4.3295E − 09	4.999	5.4312E − 09	4.997	4.8743E − 09	5.000
399	1.3534E − 10	–	1.7002E − 10	–	1.5234E − 10	–
$y(-1) = y'(1) = 0, \qquad p = p_R = 6 - 4 \times (3/4) = 3$						
N	$\delta\lambda_{5,N}$	order	$\delta\lambda_{10,N}$	order	$\delta\lambda_{20,N}$	order
49	2.1678E − 03	3.002	7.9981E − 03	2.999	1.2424E − 02	2.985
99	2.7065E − 04	3.000	1.0005E − 03	3.000	1.5693E − 03	2.999
199	3.3820E − 05	3.000	1.2505E − 04	3.000	1.9636E − 04	3.000
399	4.2273E − 06	–	1.5631E − 05	–	2.4547E − 05	–
$y'(\pm 1) = 0, \qquad p = p_R = 3$						
N	$\delta\lambda_{5,N}$	order	$\delta\lambda_{10,N}$	order	$\delta\lambda_{20,N}$	order
49	1.7360E − 03	3.001	7.4699E − 03	3.003	1.2385E − 02	2.989
99	2.1688E − 04	3.000	9.3168E − 04	3.001	1.5602E − 03	2.999
199	2.7105E − 05	3.000	1.1637E − 04	3.000	1.9510E − 04	3.000
399	3.3881E − 06	–	1.4543E − 05	–	2.4386E − 05	–
$y'(\pm 1) = y(\pm 1), \qquad p = p_R = 3$						
N	$\delta\lambda_{5,N}$	order	$\delta\lambda_{10,N}$	order	$\delta\lambda_{20,N}$	order
49	2.0295E − 03	3.002	8.1569E − 03	3.004	1.2697E − 02	2.990
99	2.5338E − 04	3.000	1.0168E − 03	3.001	1.5983E − 03	3.000
199	3.1663E − 05	3.000	1.2698E − 04	3.000	1.9983E − 04	3.000
399	3.9576E − 06	–	1.5869E − 05	–	2.4977E − 05	–

Finally, we must say that in the actual implementation we do not consider the correction terms corresponding to values of r_i and of ℓ_i in (38) that are greater than one since their contributions are surely irrelevant with respect to the others. The advantage is that for the computation of $\mu^{(N)}$ we do not need to evaluate derivatives of g_i at the endpoints of order greater than one. In this way, altogether, the cost for the application of (44) is very low since it is essentially given by the evaluations of $g_i(\pm 1)$, eventually of $g_i'(\pm 1)$ and of $\hat{z}_N(\pm 1)$ which is simple because the values of $\mathcal{R}_n(\pm 1)$ or of $\mathcal{R}_n'(\pm 1)$ are known (see (12) and (13)).

4. Numerical tests

The method described was implemented in Matlab (`ver.R2017a`). In particular, we used routines included in the open-source `Chebfun` package [7] for the computation of the matrix Q_N and we solved the generalized eigenvalue problem (9) by using the `eigs` function, with option "`SM`" for getting the ones of smallest magnitude.

TABLE 3. Order of convergence for problems with potential (46).

$y'(-1)=y(1)=0, \quad p=p_L=6-4\times(1/2)=4$						
N	$\delta\lambda_{5,N}$	order	$\delta\lambda_{10,N}$	order	$\delta\lambda_{20,N}$	order
49	6.1520E−05	3.998	7.5495E−05	3.993	6.9334E−05	3.974
99	3.8510E−06	3.999	4.7406E−06	3.999	4.4108E−06	3.997
199	2.4080E−07	4.000	2.9654E−07	4.000	2.7632E−07	4.000
399	1.5052E−08	–	1.8538E−08	–	1.7275E−08	–
$y(-1)=y'(1)=0, \quad p=p_R=6-4\times(7/8)=2.5$						
N	$\delta\lambda_{5,N}$	order	$\delta\lambda_{10,N}$	order	$\delta\lambda_{20,N}$	order
49	6.9840E−03	2.503	2.4576E−02	2.502	4.1088E−02	2.491
99	1.2317E−03	2.501	4.3385E−03	2.501	7.3081E−03	2.500
199	2.1760E−04	2.500	7.6648E−04	2.500	1.2921E−03	2.500
399	3.8460E−05	–	1.3547E−04	–	2.2839E−04	–
$y'(\pm1)=0, \quad p=p_R=2.5$						
N	$\delta\lambda_{5,N}$	order	$\delta\lambda_{10,N}$	order	$\delta\lambda_{20,N}$	order
49	5.6379E−03	2.507	2.3091E−02	2.510	4.0904E−02	2.497
99	9.9209E−04	2.502	4.0545E−03	2.503	7.2462E−03	2.501
199	1.7508E−04	2.501	7.1512E−04	2.501	1.2797E−03	2.501
399	3.0932E−05	–	1.2633E−04	–	2.2612E−04	–
$y'(\pm1)=y(\pm1), \quad p=p_R=2.5$						
N	$\delta\lambda_{5,N}$	order	$\delta\lambda_{10,N}$	order	$\delta\lambda_{20,N}$	order
49	6.4759E−03	2.506	2.5025E−02	2.510	4.2056E−02	2.498
99	1.1403E−03	2.502	4.3929E−03	2.503	7.4452E−03	2.502
199	2.0131E−04	2.501	7.7477E−04	2.501	1.3146E−03	2.501
399	3.5571E−05	–	1.3686E−04	–	2.3228E−04	–

The first results that we present confirm the statement of Theorem 3.3. In particular, we considered the problems with one of the following potentials

$$q(x) = \frac{10\,\mathrm{e}^{1-x}}{(1-x)^{3/4}(1+x)^{1/4}}, \tag{45}$$

$$q(x) = \frac{10\cos(4(1+x))}{(1+x)^{1/2}} + \frac{5\sin(4(1+x))}{(1-x)^{7/8}(1+x)^{3/4}}, \tag{46}$$

subject to one of the next four BCs

$$y'(-1)=y(1)=0, \quad y(-1)=y'(1)=0, \quad y'(\pm1)=0, \quad y'(\pm1)=y(\pm1). \tag{47}$$

In addition, we used the classical formula

$$p \approx \log_2\left(\delta\lambda_{k,N}/\delta\lambda_{k,2N+1}\right), \qquad \delta\lambda_{k,N} \equiv |\lambda_k^{(N)} - \lambda_k^{(2N+1)}|,$$

for the numerical estimate of the order of convergence (the lower index k denotes the index of the eigenvalue). The results we got for the eigenvalues of index $k = 5, 10, 20$, are listed in Table 2 for the first potential and in Table 3 for the second one. As one can see, such results are in perfect agreement with the statement of the theorem previously mentioned.

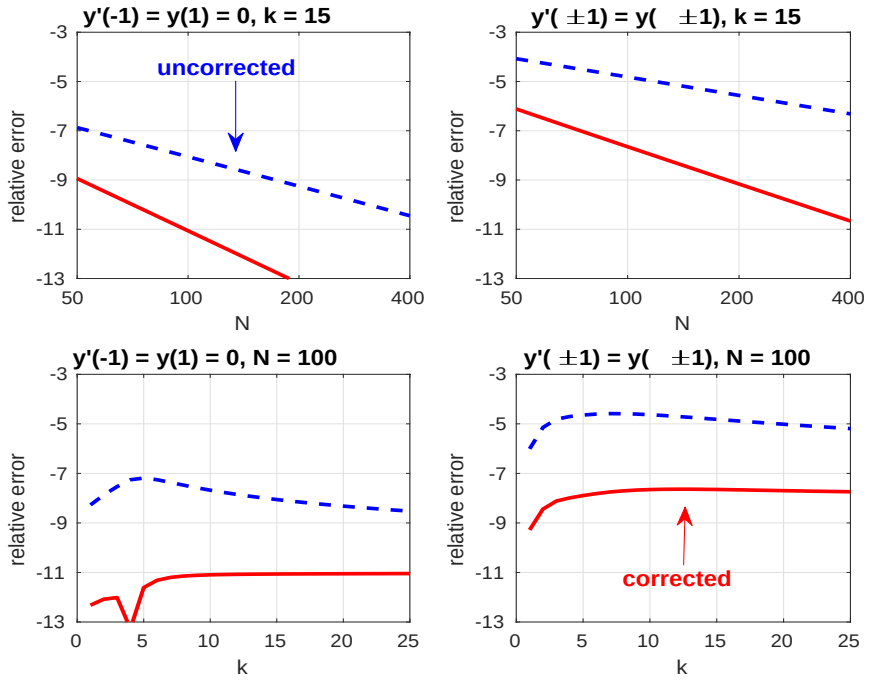

FIGURE 1. Relative errors for problems with potential (46).

Concerning the problems with q defined in (46) subject to the first or to the last BCs in (47), we applied the a posteriori correction, namely we computed also $\mu_k^{(N)}$ defined in (44). In addition, for these problems and for the subsequent ones, we evaluated the relative errors

$$\log_{10}\left(|\lambda_k^{(N)} - \bar{\lambda}_k|/|\bar{\lambda}_k|\right), \qquad \log_{10}\left(|\mu_k^{(N)} - \bar{\lambda}_k|/|\bar{\lambda}_k|\right), \tag{48}$$

by using as reference "exact" eigenvalue the values of $\bar{\lambda}_k \equiv \mu_k^{(Nt)}$ with $Nt = 5000 \gg N \geq k$. The resulting relative errors (48) have been reported in Figure 1. In more details, in the subplots at the top of such figure, the relative errors in the approximation of the fifteenth eigenvalue are plotted versus N with N ranging from 50 to 400. For the subplots at the bottom, instead, we fixed $N = 100$ and we depict the errors for the index k ranging from 1 to 25. The legend of each graphic and of the subsequent ones is dashed line and solid line for the errors in the uncorrected numerical eigenvalues and in the corrected ones, respectively. These results show that the a posteriori correction is very effective from many point of views. In fact:

- from the subplots on the bottom one deduces that for $N = 100$ and $1 \leq k \leq 25$ the gain resulting from the correction is larger than two significant digits;
- the two subplots on the top show that $\mu_{15}^{(N)}$ is always more accurate than $\lambda_{15}^{(2N)}$;
- the error in the corrected numerical eigenvalues decreases much faster with respect to N than the error in the uncorrected ones. Concerning this point,

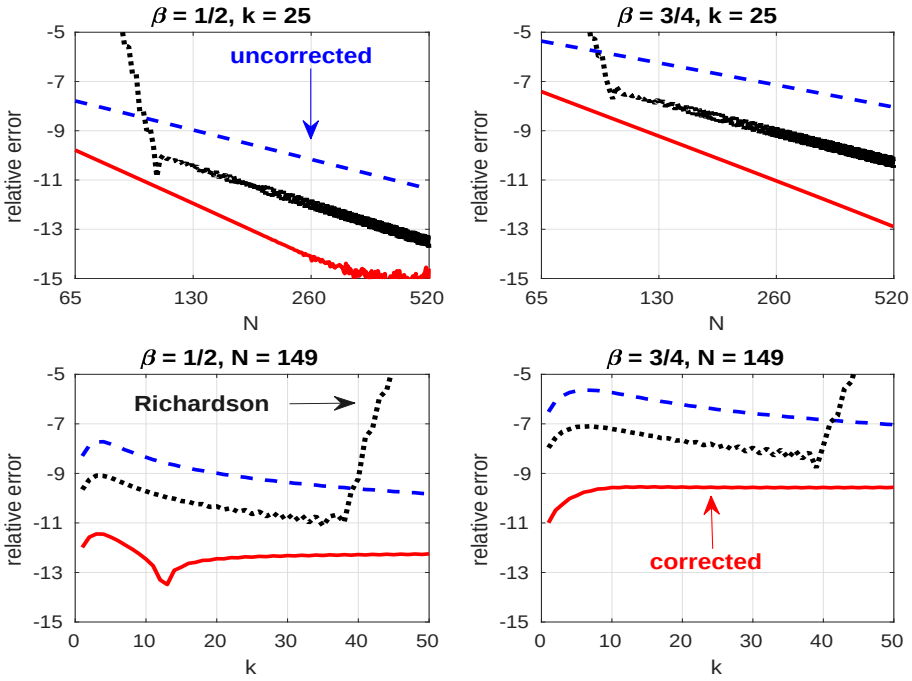

FIGURE 2. Relative errors for the symmetric problems with potential (49) subject to Neumann-Neumann BCs.

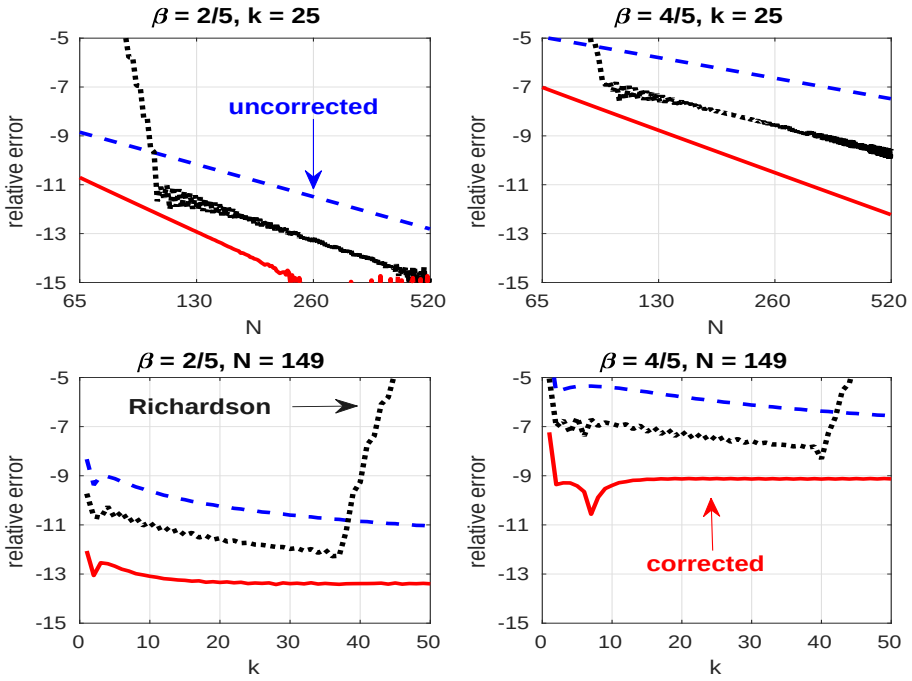

FIGURE 3. Relative errors for problems with potentials (50) subject to $y(-1) - y'(-1) = y'(1) = 0$.

we used a least-square approach to evaluate numerically the order of convergence p_μ such that

$$|\mu_k^{(N)} - \bar{\lambda}_k| = O((N+1)^{-p_\mu}).$$

For these examples, we obtained $p_\mu \approx 7$ for the problem subject to Neumann-Dirichlet BCs and $p_\mu \approx 5$ for the one subject to the unsymmetric Robin-Robin BCs.

In the following final tests, we compare the performances of our correction technique with those of the classical Richardson extrapolation given by

$$\rho_k^{(N)} \equiv \frac{2^p\,\lambda_k^{(N)} - \lambda_k^{(N-1)/2}}{2^p - 1} \approx \lambda_k, \qquad N \text{ odd},$$

where p is specified in the convergence theorem. In particular, we considered symmetric problems with potentials

$$q(x) = \frac{10}{(2-x^2)(1-x^2)^\beta}, \quad \beta = \frac{1}{2}, \frac{3}{4}, \tag{49}$$

and problems with the following not symmetric q's

$$q(x) = 5\,\frac{\cosh(x)\,(1+x)^{\frac{1}{5}} + 2\log(\frac{3}{2}+x)(1-x)^{\frac{1}{5}} + 4(1-x^2)}{(1-x^2)^\beta}, \quad \beta = \frac{2}{5}, \frac{4}{5}. \tag{50}$$

The results obtained for some BCs have been reported in Figures 2 and 3 (the errors corresponding to $\rho_k^{(N)}$ are depicted in dotted lines). As one can see, the Richardson extrapolation requires N much larger than k to improve the eigenvalue approximation, say N not smaller than $4k+1$. If this is not the case then it may deteriorates drastically the accuracy of $\lambda_k^{(N)}$. Furthermore, the improvement that we get with our low-cost method is undeniably larger than that obtained with Richardson.

Conflict of interest

The author declare that she has no conflict of interest.

References

[1] L. Aceto, P. Ghelardoni, C. Magherini, Boundary value methods as an extension of Numerov's method for Sturm-Liouville eigenvalue estimates, Appl. Numer. Math. 59 no. 7 1644-1656 (2009).

[2] L. Aceto, P. Ghelardoni, C. Magherini, BVMs for Sturm-Liouville eigenvalue estimates with general boundary conditions, JNAIAM J. Numer. Anal. Ind. Appl. Math. 4 no. 1-2 113-127 (2009).

[3] P. Amodio, G. Settanni, Reprint of Variable-step finite difference schemes for the solution of Sturm-Liouville problems, Commun. Nonlinear Sci. Numer. Simul., 21 12-21 (2015).

[4] P. B. Bailey, W. N. Everitt, A. Zettl. The SLEIGN2 Sturm-Liouville Code, ACM Trans. Math. Software, 21, 143-192 (2001). Available at: `http://www.math.niu.edu/SL2/`

[5] H. Chen, B. D. Shizgal, A spectral solution of the Sturm-Liouville equation: comparison of classical and nonclassical basis sets, J. Comput. Appl. Math., 136, 17-35 (2001).

[6] I. Çelik, Approximate computation of eigenvalues with Chebyshev collocation method, Appl. Math. Comput., 168 125-134 (2005).

[7] T. A. Driscoll, N. Hale, L. N. Trefethen, editors, Chebfun Guide, Pafnuty Publications, Oxford, 2014. Version used: 5.7.0.

[8] M. El-gamel, M. Abd El-hady, Two very accurate and efficient methods for computing eigenvalues of Sturm-Liouville problems, Appl. Math. Model. 37 5039-5046 (2013).

[9] A. Erdélyi, W. Magnus, F. Oberhettinger, F. G. Tricomi, Tables of Integral Transforms, Vol. II. Based, in part, on notes left by Harry Bateman. McGraw-Hill Book Company, Inc., New York-Toronto-London, 1954.

[10] P. Ghelardoni, C. Magherini, A matrix method for fractional Sturm-Liouville problems on bounded domain, Adv. Comput. Math. 43, 1377-1401 (2017).
[11] V. Ledoux, M. Van Daele, Matslise 2.0: a Matlab toolbox of Sturm-Liouville computations, ACM Trans. Math. Software 42, no. 4, Art. 29, 18 pp. (2016) Available at `https://sourceforge.net/projects/matslise/`
[12] V. Ledoux, Study of special algorithms for solving Sturm-Liouville and Schrödinger equations. Ph.D. Thesis, Universiteit Gent, 2007
[13] C. Magherini, A corrected spectral method for Sturm-Liouville problems with unbounded potential at one endpoint, J. Comput. Appl. Math., 364 Art. ID 112349 (2020).
[14] V. A. Marchenko, Sturm-Liouville operators and applications. Revised edition, AMS Chelsea Publishing, Providence, RI (2011).
[15] S. Pruess, C. T. Fulton, Mathematical software for Sturm-Liouville problems, ACM Trans. on Math. Software, 19, 360-376 (1993). Release 2.2 (1993-12-04). Available at `http://www.netlib.org/misc/sledge`
[16] J.D. Pryce, Numerical Solution of Sturm-Liouville Problems, Oxford: Univ. Press, London, 1993.
[17] A. G. C. P. Ramos, A. Iserles, Numerical solution of Sturm-Liouville problems via fer streamers. Numerische Mathematik, 131 no.3 541-565 (2015).
[18] J. Shen, Efficient Spectral-Galerkin Method I. Direct Solvers for the Second and Fourth Order Equations Using Legendre Polynomials, SIAM J. Sci. Comput. 15 no.6 1489-1505 (1994).
[19] A. Sidi, Asymptotic expansion of Legendre series coefficients for functions with endpoint singularities, Asymptotic Analysis 65 175-190, (2009).
[20] G. Teschl, Mathematical Methods in Quantum Mechanics with Applications to Schrödinger Operators, Providence, American Mathematical Society, 2009.
[21] A. Townsend, M. Werb, S. Olver, Fast polynomial transforms based on Toeplitz and Hankel matrices, Math. Comp. 87, 1913-1934 (2018).
[22] S. Yuan, K. Ye, C. Xiao, D. Kennedy, F. W. Williams, Solution of regular second- and fourth-order Sturm-Liouville problems by exact dynamic stiffness method analogy, J. Eng. Math. 86 157-173 (2014).
[23] Q. Yuan, Z. He, H. Leng, An improvement for Chebyshev collocation method in solving certain Sturm-Liouville problems, Appl. Math. Comput. 195 440-447 (2008).
[24] U. Yücel, Numerical approximations of Sturm-Liouville eigenvalues using Chebyshev polynomial expansions method, Cogent Math. 2, Art. ID 1045223, 13 pp. (2015).

Dipartimento di Matematica, Università di Pisa, I-56127 Pisa (Italy)
E-mail: `cecilia.magherini@unipi.it`