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Boundary Value Methods as an extension of Numerov's method for Sturm–Liouville eigenvalue estimates

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ABSTRACT

In this paper a class of Boundary Value Methods obtained as an extension of the Numerov's method is proposed for the numerical approximation of the eigenvalues of regular Sturm–Liouville problems subject to Dirichlet boundary conditions. It is proved that the error in the so obtained estimate of the kth eigenvalue behaves as $O(k^{p+1}h^{p-1/2}) + O(k^{p+2}h^p)$, where p is the order of accuracy of the method and h is the discretization stepsize. Numerical results comparing the performances of the new matrix methods with that of the corrected Numerov's method are also reported.

1. Introduction

The approximation of the eigenvalues of a regular Sturm–Liouville problem (SLP) with Dirichlet boundary conditions which, without loss of generality, can be written as

$$\begin{aligned} &-y'' + q(x)y = \lambda y, \\ &y(0) = y(\pi) = 0, \end{aligned} \tag{1}$$

is a classical problem that has led to the development of many numerical techniques. Among them, the matrix methods are based on the application of finite difference or finite element methods for reducing the SLP (1) to a generalized matrix eigenvalue problem. In this context, the most popular methods are the three-point finite difference scheme and the Numerov's method. These methods are very simple to set-up and quite cheap to implement since in both cases the involved matrices are symmetric and tridiagonal. However, the quality of the numerical approximation they provide for the kth eigenvalue deteriorates significantly as the index k increases. In view of this fact, different approaches for the treatment of the problem have been studied across the years and the most well established are based on shooting-type algorithms which require the solution of a sequence of initial value problems. These are either obtained by applying numerical methods for ordinary differential equations as done in [1,12,15] or by applying Pruess-like methods based on suitable approximations of the coefficients of the continuous problem as in [17,22,23]. In general, the shooting-type methods demand a greater effort to implement properly but, with respect to the index k, they can provide more uniformly accurate estimates of the eigenvalues. We mention that a further extension of the Pruess method has been proposed in [20].

On the other side, in the area of matrix methods, an important branch of research has been devoted to the development of suitable correction techniques for improving the accuracy of the computed eigenvalues and one of the most famous is known as asymptotic (or algebraic) correction. In the case of SLPs subject to Dirichlet boundary conditions, it was introduced

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by Anderssen, de Hoog and Paine in [21] for the three-point scheme and by Andrew and Paine in [11] for the Numerov's method. In view of its authors, sometimes, it is also called "the AAdHP correction". It is based on the observation that the leading term in the asymptotic expansion of the error in the computed eigenvalue is independent of the potential q. This fact has suggested to use the error for $q \equiv 0$, which is known in closed form, as a good estimate for the error corresponding to general q. Concerning regular SLPs involving general boundary conditions given by

$$a_1 y(0) + a_2 y'(0) = b_1 y(\pi) + b_2 y'(\pi) = 0,$$

the results reported in [21] have been extended by Anderssen and de Hoog in [6] while those reported in [11] have been more recently generalized by Andrew in [7–9]. We mention that, for both methods, the asymptotic correction can be applied at negligible extra cost also when the coefficients of the boundary conditions satisfy $a_1 a_2 = b_1 b_2 = 0$ or $a_1 b_2 = b_1 a_2 \neq 0$.

An alternative approach, with respect to the asymptotic correction, for improving the accuracy of the numerical eigenvalues provided by the Numerov's method has been proposed by Vanden Berghe and De Meyer in [25–27]. In such papers the authors have discussed a modified Numerov's scheme characterized by step-dependent coefficients determined by means of an appropriate minimization of the local error term.

In this work we consider the application of a class of symmetric Boundary Value Methods (BVMs), designed for solving second order differential equations, for approximating the eigenvalues of the SLP (1). The idea of applying BVMs for such purpose was introduced by Ghelardoni in [14] where, however, the reformulation of the continuous problem as a system of first order ordinary differential equations (ODEs) was considered. Subsequently, they were used by Aceto, Ghelardoni and Marletta in [2] in order to find an initial guess for the shooting procedure developed for approximating the eigenvalues embedded in spectral gaps. We recall that BVMs are Linear Multistep Formulas (LMFs) coupled with suitable boundary conditions instead of just initial ones as classically done. They were introduced at the beginning of the 1990s for the numerical integration of first order ODEs and the principal reference for them is the book by Brugnano and Trigiante [13]. Lately, Amodio and Iavernaro [5] have developed BVMs for solving second order differential problems of special type in their original formulation. Nevertheless, in such paper the attention was essentially devoted to the stability properties of the schemes and the principal aim was the derivation of methods having stability regions as large as possible. Here we shall deal with a class of symmetric BVMs applied to SLPs that may be considered as an extension of Numerov's method in spite of their limited stability region. In this framework, in fact, the Numerov's method can be considered as a 2-step BVM of order four. The schemes that we propose are then obtained by increasing the number of steps of the formula which allows to derive methods of arbitrarily high-order of accuracy. If the potential q is a "sufficiently" regular real-valued function, as we will always assume hereafter, then the method of order $p > 4$ applied to the SLP (1) provides an approximation of the kth eigenvalue with an error that behaves as $O(k^{p+1}h^{p-1/2}) + O(k^{p+2}h^p)$. Here $h = \pi/(N+1)$, $k = 1, 2, \ldots, N$, and $N+2$ is the number of points composing the discretization of the interval of integration. In light of this property, the new methods turn out to be competitive with respect to the corrected Numerov's one at least for the lowest index eigenvalues. In addition, there is numerical evidence that the AAdHP correction improves the eigenvalue estimates provided by the former methods and this extends the range of values of k for which they are competitive with the latter one.

The layout of this article is as follows. Section 2 is devoted to a survey of the two classical discretization methods and of the corresponding AAdHP correction technique. Section 3 introduces the class of symmetric BVMs, generalizing the Numerov's method, we shall deal with. In Section 4 the order of accuracy of the eigenvalue estimates provided by the new methods is analyzed. Section 5 briefly discusses a version of the above BVMs defined over an assigned nonuniform mesh. Finally, in Section 6 some numerical results are reported showing the possible advantages that may arise from the use of the proposed schemes.

2. Three-point scheme and Numerov's method

In this section we recall the main results concerning the two most popular matrix methods classically used for approximating the eigenvalues of the SLP (1). They are both based on the application of a difference scheme for solving a boundary value problem for the second order differential equation of special type

$$y'' = f(x, y), \quad x \in [0, \pi],$$

without recasting it as a system of two first order ODEs. In particular, by denoting with

$$x_0 = 0, \qquad x_i = x_0 + ih, \quad i = 1, \ldots, N+1, \quad h = \frac{\pi}{(N+1)}, \tag{2}$$

a uniform mesh over the time integration interval, the three-point scheme is defined by

$$\frac{y_{n-1} - 2y_n + y_{n+1}}{h^2} = f_n, \quad n = 1, 2, \ldots, N, \tag{3}$$

being y_n the numerical approximation of $y(x_n)$ and $f_n = f(x_n, y_n)$, while the Numerov's method is given by

$$\frac{y_{n-1} - 2y_n + y_{n+1}}{h^2} = \frac{1}{12}(f_{n-1} + 10f_n + f_{n+1}), \quad n = 1, 2, \ldots, N. \tag{4}$$

As it is well known, their order of accuracy is $p = 2$ for the former method and $p = 4$ for the latter one.

When applied for approximating the eigenvalues of (1), these two schemes replace the continuous problem with the following generalized matrix eigenvalue one

$$\left(-\frac{1}{h^2}T + BQ\right)\mathbf{y}^{(h)} = \lambda^{(h)} B\mathbf{y}^{(h)}, \tag{5}$$

where $\lambda^{(h)}$ denotes the numerical approximation of one of the exact eigenvalues,

$$T = \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}_{N\times N}, \qquad Q = \begin{pmatrix} q(x_1) & & & \\ & q(x_2) & & \\ & & \ddots & \\ & & & q(x_N) \end{pmatrix}. \tag{6}$$

Moreover, $B = I$, the identity matrix of size N, for the three-point scheme and

$$B = I + \frac{1}{12}T \tag{7}$$

for the Numerov's method. Obviously, for the former method the discrete problem (5) is more properly an ordinary eigenvalue one.

The error in the so obtained numerical approximation $\lambda_k^{(h)}$ for the kth exact eigenvalue λ_k is

$$\left|\lambda_k^{(h)} - \lambda_k\right| \sim O\left(k^{p+2}h^p\right), \quad k = 1, 2, \ldots, N,$$

as it can be deduced from Theorem 1 of Keller in [18], in view of the fact that the matrices $-T$ and B are both symmetric and positive definite.

In 1981, Paine et al. in [21] showed that the leading term in the asymptotic expansion of the error for the three-point scheme does not depend on the potential q. Moreover, for such method the error is known in closed form when $q \equiv 0$. They therefore suggested to use this information to correct the computed eigenvalue in the case of general q. In more details, the corrected kth eigenvalue is computed as

$$\hat{\lambda}_k^{(h)} = \lambda_k^{(h)} + \Lambda_k - \Lambda_k^{(h)}, \tag{8}$$

where Λ_k and $\Lambda_k^{(h)}$ are the kth exact and numerical eigenvalues for $q \equiv 0$, respectively. In the same paper, the authors proved that the resulting error in the kth eigenvalue is given by $|\hat{\lambda}_k^{(h)} - \lambda_k| \sim O(kh^2)$.

Later, Andrew and Paine in [11] studied the asymptotic correction technique (8) applied to the Numerov's method. For such scheme the error $\Lambda_k - \Lambda_k^{(h)}$ is known in closed form as well and it was proved that the obtained error after the correction is $O(k^3h^4)$. However, as suggested in [11], it is possible to verify numerically that in many cases the error for the corrected Numerov's method is actually $O(k^2h^4)$.

For completeness we mention that, when q is sufficiently smooth, there is numerical evidence that the approximations provided by the corrected Numerov's method can be further improved by using extrapolation, even though this requires an additional computational cost (see [10,24]).

3. A generalization of Numerov's method in the BVM framework

The schemes (3) and (4) are instances of a (2ν)-step LMF of the following type

$$\frac{y_{n-1} - 2y_n + y_{n+1}}{h^2} = \sum_{i=0}^{2\nu} \beta_i^{(\nu,2\nu)} f_{n+i-\nu}, \quad n = \nu, \nu+1, \ldots, N+1-\nu, \tag{9}$$

both with $\nu = 1$ but with different coefficients $\beta_i^{(1,2)}$. In particular, the Numerov's method is the unique one having the maximum attainable order of accuracy for a 2-step formula, i.e. $p = 4$. Here our attention will be devoted to LMFs of such type with $\nu \geqslant 1$ and coefficients $\beta_i^{(\nu,2\nu)}$ determined by requiring the formula to have the highest possible order. In this setting, the Numerov's method is therefore the one corresponding to $\nu = 1$.

In the sequel we will assume $y_0 = y_{N+1} = 0$ since our concern is the application of (9) for discretizing the SLP (1). When $\nu > 1$ it is clear that we need $2\nu - 2$ extra conditions to get the uniqueness of the discrete solution. Using the BVM approach [5,13], the *main formula* (9) is coupled with the following *initial* and *final* additional methods

$$\frac{y_{s-1} - 2y_s + y_{s+1}}{h^2} = \sum_{i=0}^{2\nu} \beta_i^{(s,2\nu)} f_i, \qquad s = 1, 2, \ldots, \nu-1, \tag{10}$$

$$\frac{y_{m-1} - 2y_m + y_{m+1}}{h^2} = \sum_{i=0}^{2\nu} \beta_i^{(s,2\nu)} f_{m-s+i}, \quad s = \nu+1, \ldots, 2\nu-1, \ m = N+1+s-2\nu, \tag{11}$$

respectively. For $s = 1, 2, \ldots, 2\nu - 1$, let

$$\boldsymbol{\alpha}^{(s,2\nu)} = \left(\alpha_0^{(s,2\nu)}, \ldots, \alpha_{2\nu}^{(s,2\nu)}\right)^T$$

be the vectors whose nonzero entries are $\alpha_s^{(s,2\nu)} = -2$ and $\alpha_{s-1}^{(s,2\nu)} = \alpha_{s+1}^{(s,2\nu)} = 1$. Clearly

$$\sum_{i=-\nu}^{\nu} \alpha_{i+\nu}^{(s,2\nu)} = 0, \qquad \sum_{i=-\nu}^{\nu} i\,\alpha_{i+\nu}^{(s,2\nu)} = 0, \tag{12}$$

so that the sth formula has at least order $2\nu + 1$ if its coefficients satisfy

$$\sum_{i=-\nu}^{\nu} i^j\,\alpha_{i+\nu}^{(s,2\nu)} - j(j-1)\sum_{i=-\nu}^{\nu} i^{j-2}\,\beta_{i+\nu}^{(s,2\nu)} = 0, \quad j = 2, \ldots, 2\nu + 2. \tag{13}$$

The order conditions (12)–(13) are obtained by applying the Taylor series expansion of the exact solution at $x = x_\nu$ instead of at $x = x_0$ as classically done. In particular, the conditions in (13) uniquely determine the $2\nu + 1$ unknown entries of the vector

$$\boldsymbol{\beta}^{(s,2\nu)} = \left(\beta_0^{(s,2\nu)}, \ldots, \beta_{2\nu}^{(s,2\nu)}\right)^T$$

as the solution of the linear system

$$\tilde{D}_{2\nu} V_{2\nu} \boldsymbol{\beta}^{(s,2\nu)} = V_{2\nu} D_{2\nu}^2 \boldsymbol{\alpha}^{(s,2\nu)}, \tag{14}$$

where

$$\tilde{D}_{2\nu} = \operatorname{diag}\big(2 \cdot 1, 3 \cdot 2, \ldots, (2\nu + 2) \cdot (2\nu + 1)\big), \tag{15}$$

$$V_{2\nu} = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ -\nu & 1-\nu & \cdots & \nu \\ \vdots & \vdots & & \vdots \\ (-\nu)^{2\nu} & (1-\nu)^{2\nu} & \cdots & \nu^{2\nu} \end{pmatrix}, \qquad D_{2\nu} = \begin{pmatrix} -\nu & & & \\ & 1-\nu & & \\ & & \ddots & \\ & & & \nu \end{pmatrix}. \tag{16}$$

In the remaining part of this section we shall discuss some properties of the just described schemes which will be useful in the sequel when speaking about their application to SLPs.

Proposition 3.1. *The proposed composite scheme* (9)–(11) *is symmetric, namely, by denoting with J the anti-identity matrix of size $2\nu + 1$, its coefficient vectors satisfy*

$$\boldsymbol{\alpha}^{(2\nu-s,2\nu)} = J\boldsymbol{\alpha}^{(s,2\nu)}, \qquad \boldsymbol{\beta}^{(2\nu-s,2\nu)} = J\boldsymbol{\beta}^{(s,2\nu)}, \quad s = 1, 2, \ldots, \nu. \tag{17}$$

Proof. The first relation is trivially satisfied by construction.

Concerning the second one, let $\tilde{\boldsymbol{\beta}}^{(s,2\nu)} = J\boldsymbol{\beta}^{(s,2\nu)}$. Then, by considering that $J^2 = I$ and by taking into account the first equation in (17), from (14) one obtains

$$\tilde{D}_{2\nu} V_{2\nu} J\tilde{\boldsymbol{\beta}}^{(s,2\nu)} = V_{2\nu} J^2 D_{2\nu}^2 J\boldsymbol{\alpha}^{(2\nu-s,2\nu)}. \tag{18}$$

It is not difficult to verify that, see (16), $JD_{2\nu}^2 J = D_{2\nu}^2$ and that $V_{2\nu} J = G V_{2\nu}$ where $G = \operatorname{diag}(1, -1, 1, \ldots, -1, 1)$. From (18), after some simple computations, one therefore gets

$$G\tilde{D}_{2\nu} V_{2\nu} \tilde{\boldsymbol{\beta}}^{(s,2\nu)} = G V_{2\nu} D_{2\nu}^2 \boldsymbol{\alpha}^{(2\nu-s,2\nu)},$$

which coincides with the linear system (14) of the order conditions for the $(2\nu - s)$th formula pre-multiplied by the non-singular matrix G. The uniqueness of the solution of such linear system implies $\tilde{\boldsymbol{\beta}}^{(s,2\nu)} = \boldsymbol{\beta}^{(2\nu-s,2\nu)}$. □

Remark 1. It is important to underline the fact that the main formula (9), i.e. the one corresponding to $s = \nu$ in (17), is a symmetric LMF. This implies that its order of accuracy is $p = 2\nu + 2$ since it must be even and not less than $2\nu + 1$. In the sequel, when speaking about the order of the composite scheme (9)–(11), we will refer to the order p of its main formula.

In Table 1 the coefficients of the main and the initial methods (9)–(10) for the BVMs with $\nu = 2, 3$, multiplied by the corresponding factor η_ν, have been reported. The coefficients of the final methods can be deduced from those of the initial ones by using (17).

Table 1
Coefficients of the main and the initial methods (9)–(10) for the BVMs with $\nu = 2, 3$.

ν	p	η_ν								
2	6	240	$\boldsymbol{\beta}^{(1,4)}$	19	204	14	4	−1		
			$\boldsymbol{\beta}^{(2,4)}$	−1	24	194	24	−1		
3	8	60480	$\boldsymbol{\beta}^{(1,6)}$	4315	53994	−2307	7948	−4827	1578	−221
			$\boldsymbol{\beta}^{(2,6)}$	−221	5862	49353	5428	213	−186	31
			$\boldsymbol{\beta}^{(3,6)}$	31	−438	6513	48268	6513	−438	31

In the next theorem we examine the existing relations between the coefficients of the main formula (9) for the methods with $(2\nu - 2)$ steps and the ones for that with (2ν) steps.

Theorem 3.2. *Let the second characteristic polynomial associated to the (2ν)-step main method (9) be*

$$\sigma_{2\nu}(z) = \sum_{j=0}^{2\nu} \beta_j^{(\nu,2\nu)} z^j. \tag{19}$$

Then,

$$\sigma_{2\nu}(z) = z\sigma_{2\nu-2}(z) - \gamma_\nu (z-1)^{2\nu}, \quad \nu = 2, 3, \ldots, \tag{20}$$

where γ_ν is the principal coefficient of the local truncation error for the $(2\nu - 2)$-step method.

Proof. Let $\mathbf{c}^{(\nu)}$ be the vector whose entries are

$$c_i^{(\nu)} = (-1)^i \binom{2\nu}{i}, \quad i = 0, 1, \ldots, 2\nu.$$

Then, from the Newton's binomial theorem the thesis holds true if

$$\boldsymbol{\beta}^{(\nu,2\nu)} = \begin{pmatrix} 0 \\ \boldsymbol{\beta}^{(\nu-1,2\nu-2)} \\ 0 \end{pmatrix} - \gamma_\nu \begin{pmatrix} c_0^{(\nu)} \\ \vdots \\ c_{2\nu}^{(\nu)} \end{pmatrix} \equiv \bar{\boldsymbol{\beta}}^{(\nu,2\nu)} - \gamma_\nu \mathbf{c}^{(\nu)}.$$

In view of the order conditions (14) for the (2ν)-step formula, which we recall uniquely determine the coefficient vector $\boldsymbol{\beta}^{(\nu,2\nu)}$, this is equivalent to prove that

$$\tilde{D}_{2\nu} V_{2\nu} \bar{\boldsymbol{\beta}}^{(\nu,2\nu)} - V_{2\nu} D_{2\nu}^2 \boldsymbol{\alpha}^{(\nu,2\nu)} = \gamma_\nu \tilde{D}_{2\nu} V_{2\nu} \mathbf{c}^{(\nu)}. \tag{21}$$

We observe that, by construction, $(\boldsymbol{\alpha}^{(\nu,2\nu)})^T = (0, (\boldsymbol{\alpha}^{(\nu-1,2\nu-2)})^T, 0)^T$. The fact that the $(2\nu - 2)$-step main formula has order 2ν, see Remark 1, implies that the left-hand side in (21) becomes

$$\tilde{D}_{2\nu} V_{2\nu} \bar{\boldsymbol{\beta}}^{(\nu,2\nu)} - V_{2\nu} D_{2\nu}^2 \boldsymbol{\alpha}^{(\nu,2\nu)} = (2\nu+2)! \gamma_\nu \mathbf{e}_{2\nu+1},$$

where $\mathbf{e}_{2\nu+1}$ is the last unit vector in $\mathbb{R}^{2\nu+1}$. Concerning the right-hand side in (21), it is known that

$$V_{2\nu} = P^{-\nu} S D_f P^T, \qquad \mathbf{c}^{(\nu)} = P^{-T} \mathbf{e}_{2\nu+1},$$

being P the Pascal matrix of size $2\nu + 1$, $D_f = \mathrm{diag}(0!, 1!, \ldots, (2\nu)!)$ and S the unit lower triangular matrix whose entries are the Stirling numbers of second kind [4]. Considering that $P^{-\nu}$ is a unit lower triangular matrix too and (15), one therefore obtains

$$\tilde{D}_{2\nu} V_{2\nu} \mathbf{c}^{(\nu)} = \tilde{D}_{2\nu} P^{-\nu} S D_f \mathbf{e}_{2\nu+1} = (2\nu)! \tilde{D}_{2\nu} P^{-\nu} S \mathbf{e}_{2\nu+1} = (2\nu+2)! \mathbf{e}_{2\nu+1},$$

which completes the proof. □

It is quite evident that the previous result implies $\gamma_\nu = -\beta_0^{(\nu,2\nu)}$. From Table 1 one deduces $\gamma_2 = \frac{1}{240}$ and $\gamma_3 = -\frac{31}{60480}$.

4. Eigenvalue estimates and related convergence analysis

The application of the (2ν)-step BVM (9)–(11) to the SLP (1) produces a generalized eigenvalue problem having the same form as (5), where the matrices T and Q are defined in (6), namely they coincide with the ones of the Numerov's method. The matrix B, instead, is now given by

$$B = \begin{pmatrix}
\beta_1^{(1)} & \cdots & \beta_\nu^{(1)} & \cdots & \beta_{2\nu-1}^{(1)} & \beta_{2\nu}^{(1)} & & & \\
\vdots & & \vdots & & \vdots & \vdots & & & \\
\beta_1^{(\nu-1)} & \cdots & \beta_\nu^{(\nu-1)} & \cdots & \beta_{2\nu-1}^{(\nu-1)} & \beta_{2\nu}^{(\nu-1)} & & & \\
\beta_1^{(\nu)} & \cdots & \beta_\nu^{(\nu)} & \cdots & \beta_1^{(\nu)} & \beta_0^{(\nu)} & & & \\
\beta_0^{(\nu)} & \beta_1^{(\nu)} & \cdots & \beta_\nu^{(\nu)} & \cdots & \beta_1^{(\nu)} & \beta_0^{(\nu)} & & \\
 & \ddots & \ddots & & \ddots & & \ddots & \ddots & \\
 & & \beta_0^{(\nu)} & \beta_1^{(\nu)} & \cdots & \beta_\nu^{(\nu)} & \cdots & \beta_1^{(\nu)} & \beta_0^{(\nu)} \\
 & & & \beta_0^{(\nu)} & \beta_1^{(\nu)} & \cdots & \beta_\nu^{(\nu)} & \cdots & \beta_1^{(\nu)} \\
 & & & \beta_{2\nu}^{(\nu-1)} & \beta_{2\nu-1}^{(\nu-1)} & \cdots & \beta_\nu^{(\nu-1)} & \cdots & \beta_1^{(\nu-1)} \\
 & & & \vdots & \vdots & & \vdots & & \vdots \\
 & & & \beta_{2\nu}^{(1)} & \beta_{2\nu-1}^{(1)} & \cdots & \beta_\nu^{(1)} & \cdots & \beta_1^{(1)}
\end{pmatrix}_{N\times N}, \tag{22}$$

where (17) has been taken into account and the second upper index for the coefficients β, denoting the stepnumber of the formula, has been omitted for the sake of simplicity. From now on, we shall always assume that B is invertible.

The study of the error in the eigenvalue approximations provided by such method is based on the analysis of the behavior of the associated local truncation error.

Let λ be an eigenvalue of (1) and $y(x)$ be the corresponding eigenfunction. We define the vector $\mathbf{y}$ whose entries are the projections of $y(x)$ over the uniform mesh (2), i.e.

$$y_j = y(x_j), \quad j = 1, 2, \ldots, N.$$

In this notation, the local truncation error $\boldsymbol{\tau}$ is given by the vector

$$\boldsymbol{\tau} = -\frac{1}{h^2} T\mathbf{y} + BQ\mathbf{y} - \lambda B\mathbf{y},$$

whose entries are

$$\tau_j = \begin{cases} \omega_\nu h^p y^{(p+2)}(\xi_j), & j = \nu, \nu+1, \ldots, N-\nu+1, \\ \omega_j h^{p-1} y^{(p+1)}(\xi_j), & \text{otherwise}, \end{cases} \tag{23}$$

where $\omega_j \in \mathbb{R}$ is the principal error coefficient of the jth formula. In particular, $\omega_\nu = \gamma_{\nu+1}$ (see Theorem 3.2) and $\omega_j = -\omega_{N+1-j}$, $j = 1, \ldots, \nu-1$, by virtue of (17).

We recall that the analysis of convergence of a generic numerical procedure is always carried out by assuming that the infinite precision arithmetic is used. In particular, in this context, this implies that, see (5), the approximations $\lambda^{(h)}$ of the exact eigenvalues λ of (1) coincide with the eigenvalues of the matrix

$$M_h = -\frac{1}{h^2} B^{-1} T + Q. \tag{24}$$

The first step in such analysis of convergence is constituted by the following result proved in [3].

Theorem 4.1. *Let us assume that the matrix M_h is diagonalizable and let U_h be the corresponding matrix of eigenvectors normalized to be of unit length. Let λ, $\mathbf{y}$ and $\boldsymbol{\tau}$ be as above. Then*

$$\left|\lambda - \lambda^{(h)}\right| = \inf_{\mu\in\sigma(M_h)} |\lambda - \mu| \leqslant \frac{\operatorname{cond}(U_h)\|B^{-1}\|\|\boldsymbol{\tau}\|}{\|\mathbf{y}\|}, \tag{25}$$

where $\sigma(M_h)$ denotes the spectrum of M_h and $\operatorname{cond}(U_h)$ is the condition number of U_h.

It is worth to note that the assumption on the matrix M_h made in the previous theorem seems to be reasonable having the SLP simple eigenvalues and thinking that M_h is a consistent discretization of the continuous problem.

From (25) it follows that the error in the approximation of the eigenvalues does have the same asymptotic behavior of the local truncation error (associated with the method and with the exact eigenfunction) provided $\operatorname{cond}(U_h)$ and $\|B^{-1}\|$ are

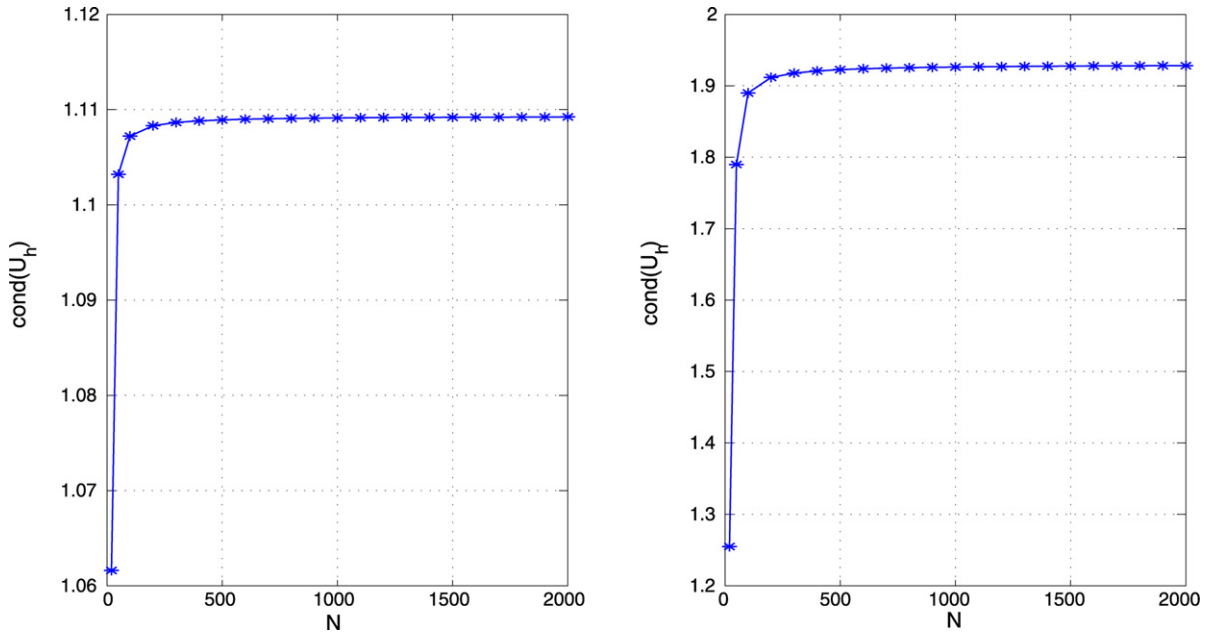

Fig. 1. Condition number of U_h for the (2ν)-step methods (9)–(11), with $\nu = 2$ (left) and $\nu = 3$ (right).

bounded independently of N. For the composite scheme (9)–(11) a theoretical analysis of the condition number of U_h turns out to be rather difficult. However, in view of many numerical experiments we have carried out by using the Euclidean norm, we can conjecture the existence of such upper bound. As an example, in Fig. 1 the obtained results for the methods with four and six steps (see Table 1) applied to the SLP (1) with potential $q(x) = -40\cos(2x-\pi) + (20\sin(2x-\pi))^2$, i.e. the one defining the Coffey–Evans problem [24], are reported.

On the other hand, the following considerations on the structure of B allow to derive some results concerning the behavior of $\|B^{-1}\|$ with respect to N. First of all, we observe that the matrix $B \equiv B^{(\nu)}$ can be decomposed as

$$B^{(\nu)} = B_T^{(\nu)} + E_0^{(\nu)}, \tag{26}$$

where $B_T^{(\nu)}$ is the Toeplitz matrix whose *symbol* is $\sigma_{2\nu}(z)/z^\nu$ (see (19)), [13]. The nonzero entries of the remainder matrix $E_0^{(\nu)}$ do not depend on N and are localized in the two submatrices of size $(\nu-1)\times(2\nu)$ positioned in its upper-left and lower-right corners, respectively. Note that for the Numerov's method, i.e. when $\nu = 1$, $B^{(1)} = B_T^{(1)}$ (see (7)) since such scheme does not require any additional formula. In the next lemma, we focus the attention on $B_T^{(\nu)}$ showing a useful property of the same that will be used in the sequel.

Lemma 4.2. *The matrix $B_T^{(\nu)}$ in* (26) *can be decomposed as*

$$B_T^{(\nu)} = p_\nu(T) + E_1^{(\nu)}, \tag{27}$$

where $p_\nu(\zeta)$ is a polynomial of degree ν satisfying the following recurrence relation:

$$\begin{cases} p_0(\zeta) = 1, \\ p_\nu(\zeta) = p_{\nu-1}(\zeta) - \gamma_\nu \zeta^\nu, \quad \nu = 1, 2, \ldots, \end{cases}$$

being $\gamma_1 = -\frac{1}{12}$ and γ_ν the principal error coefficient of the $(2\nu-2)$-step main formula for $\nu > 1$. The remainder matrix $E_1^{(\nu)}$ has the same structure of $E_0^{(\nu)}$ in (26) *with nonzero entries independent of its dimension.*

Proof. The proof is by induction. When $\nu = 1$ the thesis is trivially verified by construction with $E_1^{(1)}$ the zero matrix (see (7)). Let us assume that it holds true for $\nu - 1$ and let us prove it for ν. From (20) one obtains that the symbol associated to $B_T^{(\nu)}$ satisfies

$$\frac{\sigma_{2\nu}(z)}{z^\nu} = \frac{\sigma_{2\nu-2}(z)}{z^{\nu-1}} - \gamma_\nu \left(\frac{(z-1)^2}{z}\right)^\nu.$$

We observe that the first term on the right hand-side of the previous equality is the symbol of $B_T^{(\nu-1)}$ and that the second one is the symbol associated to a Toeplitz matrix which can be written as $\gamma_\nu T^\nu - E_2^{(\nu)}$. Once again, one quite simply verifies

Table 2
Values of $\hat{\mu}_\nu$, $\mu_1(F_\nu)$ and δ_ν for $\nu = 1, 2, 3, 4$.

ν	$\hat{\mu}_\nu$	$\mu_1(F_\nu)$	δ_ν
1	0.4444	0	1.5
2	0.3600	−0.0133	1.6983
3	0.3217	−0.0657	1.9764
4	0.2990	−0.1761	2.8525

that the remainder matrix $E_2^{(\nu)}$ has the same characteristics of $E_0^{(\nu)}$ given in (26). All these considerations, together with the induction hypothesis, lead to

$$B_T^{(\nu)} = B_T^{(\nu-1)} - \gamma_\nu T^\nu + E_2^{(\nu)} = p_{\nu-1}(T) - \gamma_\nu T^\nu + E_1^{(\nu-1)} + E_2^{(\nu)}$$
$$\equiv p_\nu(T) + E_1^{(\nu)}. \qquad \square$$

From (26) and (27) one readily deduces that

$$B = p_\nu(T) + E_\nu, \qquad E_\nu \equiv E_0^{(\nu)} + E_1^{(\nu)}. \tag{28}$$

This constitutes the starting point of the following result.

Lemma 4.3. *Let T be the tridiagonal matrix given in* (6) *and B the coefficient matrix defined in* (22) *for the (2ν)-step BVM. Moreover, let*

$$F_\nu = p_\nu(T)E_\nu^T + E_\nu p_\nu(T) + E_\nu E_\nu^T, \tag{29}$$

see (28)*, and*

$$\hat{\mu}_\nu = \min_{\zeta\in[-4,0]} p_\nu^2(\zeta).$$

Then, by denoting with $\mu_1(C)$ the minimum eigenvalue of a generic square matrix C, one has that if $N \geqslant 6\nu$

(i) *$\mu_1(F_\nu)$ is independent of N;*
(ii) *$\hat{\mu}_\nu \leqslant \mu_1(p_\nu^2(T))$ for each N;*
(iii) *if $\hat{\mu}_\nu + \mu_1(F_\nu) > 0$ then $\|B^{-1}\|_2 \leqslant (\hat{\mu}_\nu + \mu_1(F_\nu))^{-1/2} \equiv \delta_\nu$.*

Proof. The first statement is a direct consequence of the structure of the two matrices $p_\nu(T)$ and E_ν. In particular: $p_\nu(T)$ is a symmetric banded matrix of bandwidth $2\nu + 1$ since T is a symmetric tridiagonal matrix and $p_\nu(\cdot)$ is a polynomial of degree ν; the remainder matrix E_ν has the same characteristics of $E_0^{(\nu)}$ and $E_1^{(\nu)}$. From these considerations and (29), by means of some linear algebra, one deduces that if $N \geqslant 6\nu$, F_ν is a block diagonal matrix having only the first and the last block not equal to zero. Moreover, the size of such two blocks is 3ν and their entries are constant with respect to N. This obviously implies that $\mu_1(F_\nu)$ is independent of N.

The second result follows from the fact that the eigenvalues of T lie in the interval $[-4, 0]$ for each N since they are given by

$$s_k = -4\sin^2\left(\frac{k\pi}{2N+2}\right), \quad k = 1, 2, \ldots, N. \tag{30}$$

Finally, the third statement holds true if the spectral radius of $(BB^T)^{-1}$ has an upper bound not depending on N. This is equivalent to the fact that the eigenvalues of BB^T have a strictly positive lower bound. We observe that from (28) one gets

$$BB^T = \big(p_\nu(T) + E_\nu\big)\big(p_\nu(T) + E_\nu\big)^T = \big(p_\nu(T)\big)^2 + F_\nu.$$

Consequently, the lower bound we are looking for is given by $\hat{\mu}_\nu + \mu_1(F_\nu)$ which is positive by assumption. In fact, from (i)–(ii) and the Weyl Theorem [16, Section 4.3.1], which can be applied since $p_\nu^2(T)$ and F_ν are both symmetric, it results

$$\hat{\mu}_\nu + \mu_1(F_\nu) \leqslant \mu_1\big(p_\nu^2(T)\big) + \mu_1(F_\nu) \leqslant \mu_1(BB^T).$$

From these inequalities the third statement follows. $\square$

In Table 2 the numerically computed values of $\hat{\mu}_\nu$ and $\mu_1(F_\nu)$ are quoted for $\nu = 1, 2, 3, 4$. As one can see, the corresponding methods satisfy the hypothesis in the third statement of the previous lemma. In the same table we have therefore also listed the relative bound δ_ν for $\|B^{-1}\|_2$.

The following theorem completes the analysis of convergence for the BVM (9)–(11) applied for approximating the eigenvalues of the SLP (1).

Theorem 4.4. *Let λ_k be the kth exact eigenvalue of the SLP* (1) *and $\lambda_k^{(h)}$ be the corresponding numerical eigenvalue provided by the* (2ν)*-step BVM* (9)–(11)*, with $\nu > 1$. Moreover, let U_h be as in Theorem* 4.1 *and B the coefficient matrix* (22)*. Then, if* $\mathrm{cond}(U_h)$ *and* $\|B^{-1}\|$ *are bounded independently of N in Euclidean norm and if kh is "sufficiently" small, one has*

$$\left|\lambda_k^{(h)} - \lambda_k\right| \sim O\left(k^{p+1}h^{p-1/2}\right) + O\left(k^{p+2}h^p\right), \quad p = 2\nu + 2.$$

Proof. From the assumptions on $\mathrm{cond}(U_h)$ and $\|B^{-1}\|$ (the latter surely verified if so is the hypothesis of the third statement in Lemma 4.3), and from Theorem 4.1 it follows that there exists a constant C independent of N and of the index k of the eigenvalue such that

$$\left|\lambda_k^{(h)} - \lambda_k\right| \leqslant C\frac{\|\boldsymbol{\tau}_k\|_2}{\|\mathbf{y}_k\|_2} = C\frac{\|\sqrt{h}\boldsymbol{\tau}_k\|_2}{\|\sqrt{h}\mathbf{y}_k\|_2}.$$

Here $\mathbf{y}_k$ is the projection of the kth eigenfunction over the uniform mesh and $\boldsymbol{\tau}_k$ is the corresponding local truncation error. As proved in [21, Lemma 2.1], it is known that the kth eigenfunction $y_k(x)$ satisfies

$$y_k(x) = \sin(kx) + e_k(x),$$

where $e_k^{(j)}(x) \sim O(k^{j-1})$, $j = 0, 1, 2, \ldots$. This implies that $\|\sqrt{h}\mathbf{y}_k\|_2 \sim O(1)$. Moreover, from (23), by taking into account that p is even, one gets that the jth component of $\boldsymbol{\tau}_k$ satisfies

$$|\tau_j| \leqslant \begin{cases} |\omega_\nu| k^{p+2}h^p |\sin(k\xi_j)| + O(k^{p+1}h^p), & j = \nu, \ldots, N-\nu+1, \\ \hat{\omega}k^{p+1}h^{p-1}|\cos(k\xi_j)| + O(k^p h^{p-1}), & \text{otherwise}, \end{cases}$$

where $\hat{\omega} = \max_{j=1,\ldots,\nu-1}|\omega_j|$. The vector $\boldsymbol{\tau}_k$ can be therefore split as $\boldsymbol{\tau}_k = \boldsymbol{\tau}_k^{(a)} + \boldsymbol{\tau}_k^{(m)}$, with $\boldsymbol{\tau}_k^{(a)} = (\tau_1, \ldots, \tau_{\nu-1}, 0, \ldots, 0, \tau_{N-\nu+2}, \ldots, \tau_N)^T$. By considering that the number of nonzero entries of such vector is independent of N (i.e. of h), it follows that

$$\|\sqrt{h}\boldsymbol{\tau}_k\|_2 \leqslant \left\|\sqrt{h}\boldsymbol{\tau}_k^{(a)}\right\|_2 + \left\|\sqrt{h}\boldsymbol{\tau}_k^{(m)}\right\|_2 \sim O\left(k^{p+1}h^{p-1/2}\right) + O\left(k^{p+2}h^p\right)$$

and hence the thesis. □

It is important to underline the fact that the lower order of convergence of the chosen additional methods, with respect to that of the main formula, may affect only the accuracy of the estimates for the first eigenvalues.

Remark 2. An alternative generalization of the Numerov's scheme is the BVM obtained by considering as coefficient matrix $B = p_\nu(T)$, i.e. by neglecting in (28) the remainder matrix E_ν. This corresponds to couple the same main formula with additional ones having a very low order of convergence which often leads to a significant loss of accuracy in the estimate of many eigenvalues. However, this does not happen for the potential $q \equiv 0$. In fact, in this case, such method approximates the SLP eigenvalues by those of the matrix $-\frac{1}{h^2}p_\nu(T)^{-1}T$ given by

$$\tilde{\lambda}_k = \frac{1}{h^2}\frac{s_k}{\sum_{i=0}^{\nu}\gamma_i s_k^i}, \quad \gamma_0 \equiv -1,$$

where s_k is defined in (30). By means of some technical computations, here omitted for brevity, it is possible to prove that $\tilde{\lambda}_k = k^2 + O(k^{p+2}h^p)$.

5. BVMs with variable stepsize

From the analysis of convergence carried out in the previous section, it can be deduced that the new schemes are competitive with respect to the corrected Numerov's method when one is interested in getting an accurate estimate of the eigenvalues not limited only to the first few ones. This fact is confirmed by the numerical results that we are going to present in Section 6.

However, when the order p of the applied BVM increases, it may happen that some $\lambda_k^{(h)}$ turn to be complex also in the case of $q \equiv 0$. Independently of N, this drawback seems to be limited to a very small number, say one or two, of complex conjugate pairs. Moreover, having ordered the eigenvalues with increasing real part, their index k appears to be always greater than $N/2$ so that, as it is well known, they belong to the range of poorly accurate eigenvalue estimates provided by a matrix method. Anyway, this unforeseen result is in contrast with the peculiarity of a regular SLP with a real-valued potential q of having a real spectrum.

In view of the decomposition of the coefficient matrix B given in (28) this incongruity is due to the presence of the remainder matrix E_ν whose entries are essentially related to the auxiliary methods (10)–(11). In fact, by neglecting E_ν and by replacing B with $p_\nu(T)$ in (24), one would obtain a symmetric matrix M_h.

In order to get a discrete problem having the same qualitative properties of the continuous one, it is therefore necessary to reduce the effect of the additional methods on the whole composite scheme. A possible strategy consists in the refinement of the mesh near the extremes of the interval of integration as suggested in [13, Chapter 11]. Even thought different choices are possible, the set of nodes we have decided to use for building the (2ν)-step method satisfies

$$x_0 = 0, \quad x_i = x_{i-1} + h_i, \quad i = 1, 2, \ldots, N+1, \quad x_{N+1} = \pi, \tag{31}$$

where

$$\begin{cases} h_1 < h_2 < \cdots < h_\nu, \\ h_i = h_\nu, \quad i = \nu+1, \ldots, N-\nu+1, \\ h_i = h_{N-i+2}, \quad i = N-\nu+2, \ldots, N+1. \end{cases} \tag{32}$$

It is worth to note that such mesh is symmetric with respect to the midpoint of $[0, \pi]$. The LMFs occurring in the definition of the new BVM are constructed by retaining the use of a three-point formula for the discretization of the second order derivative of the eigenfunction. The remaining coefficients are then determined by imposing the highest possible order for each formula.

The numerical approximations of the SLP eigenvalues provided by the new BVM are now given by the eigenvalues of the matrix

$$M_V = -\frac{1}{h_\nu^2} B_V^{-1} T_V + Q_V,$$

where B_V, T_V and Q_V are the analogues of the matrices B, T and Q, given in (22) and (6), respectively, and B_V is assumed to be invertible.

By using a set of nodes derived from those of the Gauss–Legendre–Lobatto and of the Gauss–Chebyschev–Lobatto $(2\nu+1)$-point quadrature formulas, this strategy seems to be successful to overcome the problem of the emergence of numerical complex eigenvalues. More precisely, the nonuniform mesh (31) that we have considered is constructed starting from the following one

$$\hat{x}_0 = -1, \quad \hat{x}_i = \hat{x}_{i-1} + \hat{h}_i, \quad i = 1, 2, \ldots, N+1,$$

where $\hat{x}_i$, $i = 0, \ldots, \nu$, are the first $\nu+1$ nodes of one of the previously mentioned quadrature formulas; the remaining $\hat{x}_i$ are determined by imposing the stepsizes $\hat{h}_i$, $i > \nu$, to satisfy the properties given in (32), obviously via the formal substitution of h_i with $\hat{h}_i$. The mesh points (31) are then obtained by scaling and shifting the nodes $\hat{x}_i$ so that they are defined over the interval $[0, \pi]$. In the sequel we shall refer to these two meshes as the GLL and the GCL mesh, respectively.

Concerning the analysis of convergence of the so obtained approximations $\lambda_k^{(h_\nu)}$ of the SLP eigenvalues, similarly to what we have done in the case of the uniform mesh, we conjecture that the matrix M_V is diagonalizable and that the condition number of the corresponding eigenvector matrix is bounded with respect to N. Moreover, we assume that $\|B_V^{-1}\|$ is limited as well. These properties of M_V and B_V are confirmed by the results of the numerical experiments we have conducted with several potentials q.

Under these assumptions, arguments analogous to those used in Section 4 allow to prove that

$$\left|\lambda_k^{(h_\nu)} - \lambda_k\right| \sim O\left(k^{p+1} h_\nu^{p-1/2}\right) + O\left(k^{p+2} h_\nu^p\right), \quad k = 1, 2, \ldots, N.$$

6. Numerical results

The described BVMs have been applied to several SLPs with the aim of comparing their performances with that of the corrected Numerov's method in the approximation of the SLP eigenvalues. In this section we report some representative results obtained for some classical potentials. The numerical eigenvalues $\lambda_k^{(h)}$ have been computed by using the MATLAB command EIG for each test and the accuracy of the so obtained approximations has been evaluated by considering as "exact" the eigenvalues λ_k provided by the MATSLISE software package [19]. We take as premise that the reported comparisons are all based on the number N of mesh points alone. A more deepened comparison should take into account that for the higher order method the matrix B in (22) has a larger bandwidth. This leads to an increase of the computational cost whose exact quantification is however rather difficult since strictly related to the used routine of linear algebra and to the optimizations therein introduced.

The first results that we present refer to the SLP (1) with $q(x) = (0.1 + x)^{-2}$, [21]. In Fig. 2, the error $|\lambda_k^{(h)} - \lambda_k|$ for the 6-step BVM of order 8 with uniform mesh (dashed line) is compared with that of the corrected Numerov's method (dashdot line) since the asymptotic correction can be operated for the latter method with a negligible extra cost. More precisely, such figure consists of four plots corresponding to the approximation of the kth eigenvalue with $k = 10, 20, 30, 40$, respectively, for increasing values of N (i.e. for $h \to 0$). As one can see from the first two subplots, the 6-step BVM turns out to be competitive with respect to the corrected Numerov's scheme if one is interested in finding an accurate approximation of the first eigenvalues. In fact, the former method requires a considerable smaller number of mesh points with respect to the latter one for an a priori prescribed sufficiently high accuracy. For example, if an estimate of the 20th eigenvalue

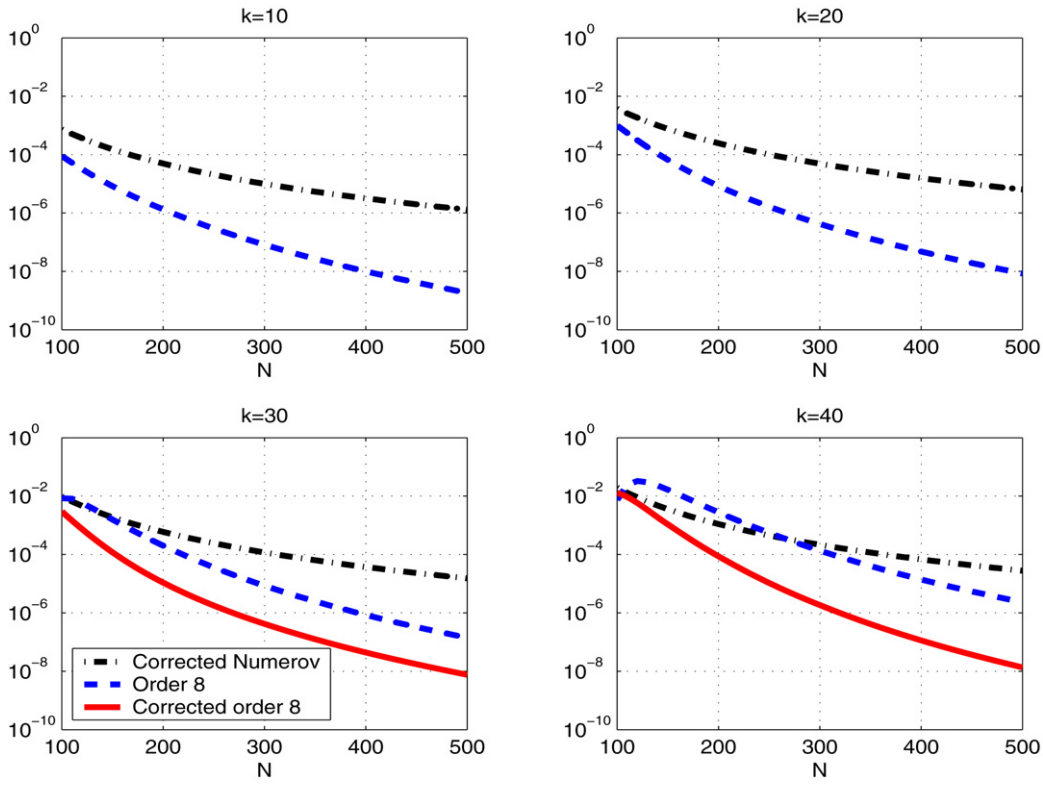

Fig. 2. Errors in the approximations of λ_k for $q(x) = (0.1 + x)^{-2}$ and $k = 10, 20, 30, 40$.

with an error of order 10^{-5} is required, the proposed BVM provides it by using $N \simeq 200$, while the corrected Numerov's method needs $N \simeq 450$. We remark that this fact is in perfect agreement with the result of Theorem 4.4 and the theory developed in [11] considering that, in such case, kh is "sufficiently" small. However, as k increases the applied BVM looses the competitiveness with respect to the corrected Numerov's method. This is not so surprising in view of the previously mentioned theoretical results. Nevertheless, the application of the asymptotic correction technique to the used BVM leads to a conspicuous improvement of the accuracy of the eigenvalue estimates provided by such method. This allows to recover their competitiveness for a longer string of eigenvalues as confirmed by the numerical results reported in the last two subplots of Fig. 2, where the error corresponding to the corrected BVM is drawn in solid line. We must say that, at least for the time being, the AAdHP correction is operated by computing the numerical eigenvalues for $q \equiv 0$. However, the corresponding computational cost can be reduced by taking into account that the coefficient matrices of the considered BVMs are centrosymmetric [28].

Using the same notations adopted for the just discussed example, in Fig. 3 we have plotted the errors in the eigenvalue estimates for the Coffey–Evans problem [24] having potential $q(x) = -40\cos(2x - \pi) + (20\sin(2x - \pi))^2$. Here we have applied the 6-step BVM defined over the GLL nonuniform mesh described in Section 5. It is evident that comments similar to those made for the previous example apply also in this case.

It is worth to mention that, for both the previous examples, we have observed that the BVM schemes introduced in this paper, with a suitably chosen order of accuracy, provide positive results also with respect to the corrected Numerov's method improved with one extrapolation.

The aim of the last example is to compare the performances of the proposed BVMs, after the asymptotic correction, as their order of accuracy increases. In particular, the results reported in Fig. 4 refer to the SLP (1) with $q(x) = \exp(x)$ and to the methods defined over the GCL nonuniform mesh with $N = 250$. As one can see the new schemes turn out to be competitive with respect to the corrected Numerov's method for the first eigenvalues. Moreover, the higher the order of the method the longer the string of eigenvalues for which such competitiveness persists.

7. Conclusions

The proposed BVMs (9)–(11) for computing the eigenvalues of regular SLPs subject to Dirichlet boundary conditions have provided positive results in terms of their competitiveness with respect to the Numerov's method. By virtue of this fact, an interesting topic for future investigation seems to be the extension of the schemes here considered to the case of SLPs with more general boundary conditions.

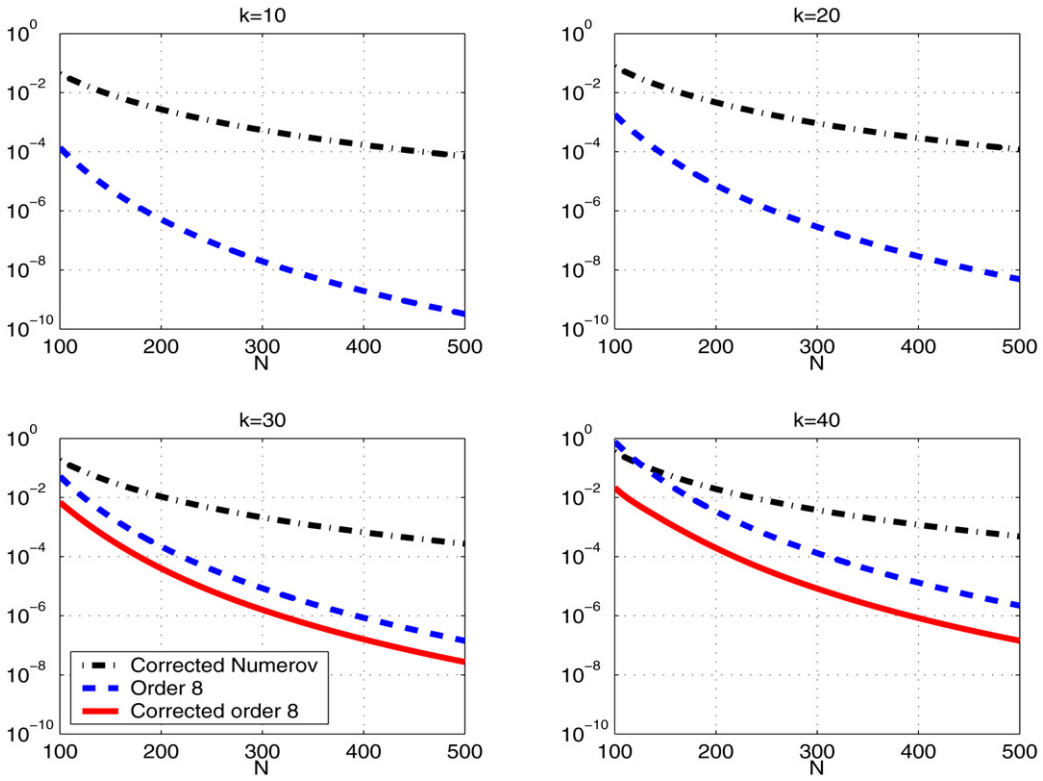

Fig. 3. Errors in the approximations of λ_k for $q(x) = -40\cos(2x-\pi) + (20\sin(2x-\pi))^2$, $k = 10, 20, 30, 40$, and the BVMs defined on the GLL nonuniform mesh.

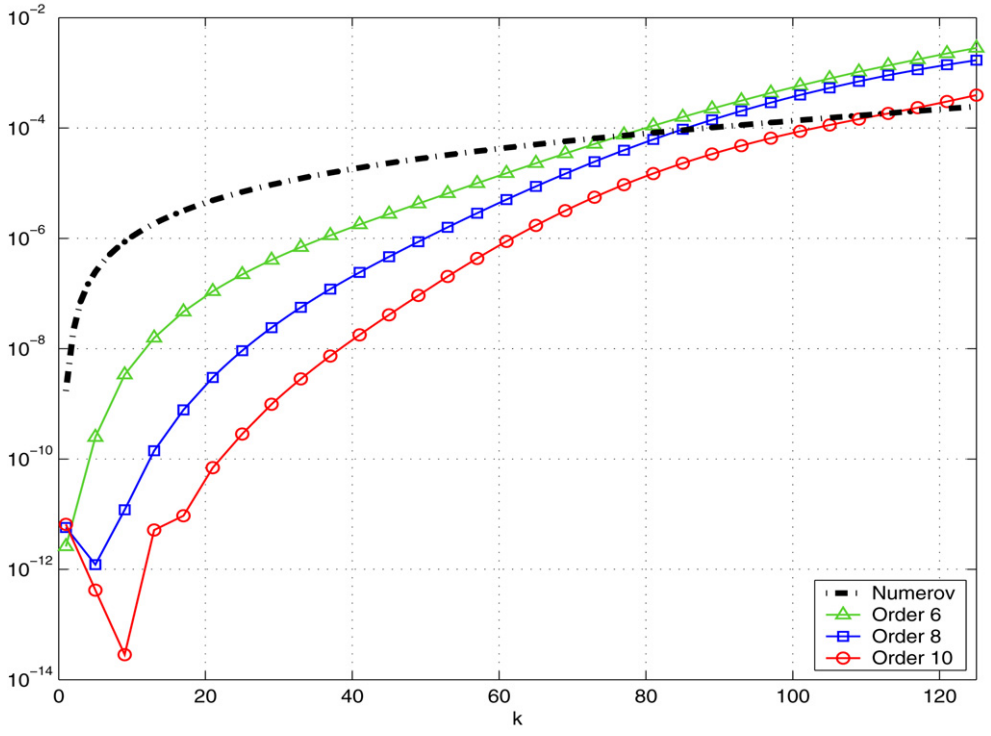

Fig. 4. Errors in the approximations of λ_k for $q(x) = \exp(x)$, $N = 250$ and the BVMs defined on the GCL nonuniform mesh.

In addition, issue remains concerning the analysis of convergence for the error in the eigenvalue estimates obtained after the application of the AAdHP correction technique.

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