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BVMs for Sturm-Liouville eigenvalue estimates with general boundary conditions[1]

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Dedicated to Prof. J.C. Butcher on the occasion of his 75th birthday

Abstract: Recently, a class of Boundary Value Methods (BVMs) has been introduced for the estimation of the eigenvalues of Sturm-Liouville problems with Dirichlet boundary conditions. The aim of this paper is to extend the application of such BVMs to problems with boundary conditions of general form and to compare the approximations obtained with those given by the corrected Numerov method.

Keywords: Sturm-Liouville problems, Eigenvalues, Boundary Value Methods.

Mathematics Subject Classification: 65L10, 65L15, 34L16

1 Introduction

This paper is devoted to the approximation of the eigenvalues of a regular Sturm-Liouville problem (SLP) given by the equation

$$-y'' + q(x)y = \lambda y\,, \quad x \in [0,\pi]\,, \tag{1}$$

subject to general boundary conditions

$$\begin{aligned} a_1 y(0) - a_2 y'(0) &= 0\,, \\ b_1 y(\pi) - b_2 y'(\pi) &= 0\,, \end{aligned} \tag{2}$$

where $|a_1| + |a_2| \neq 0$ and $|b_1| + |b_2| \neq 0$.
Many numerical techniques have been developed across the years to achieve this aim and among them the so-called *matrix methods* constitute one of the most popular family of schemes. They are based on the application of finite difference or finite element methods for reducing the SLP (1)-(2) to a matrix eigenvalue problem. In particular, the first studies were conducted for SLPs with Dirichlet boundary conditions

$$y(0) = y(\pi) = 0, \tag{3}$$

by applying the three-point scheme and the Numerov method. It is known that the error in the approximation of the kth eigenvalue provided by these two methods asymptotically behaves as

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$O(k^4h^2)$ and $O(k^6h^4)$, respectively, where h denotes the discretization stepsize. In order to improve the accuracy of such approximations, the classical extrapolation technique may be conveniently applied. Nevertheless, to this aim, the most commonly used technique is the asymptotic correction which makes use of the error for $q \equiv 0$, known in closed form, as a "good" estimate of the error for a generic potential q. This technique, described in more detail in the following section, has been introduced by Paine, de Hoog and Anderssen in [11] for the three-point scheme and by Andrew and Paine in [7] for the Numerov method. In view of its authors, it is sometimes also called the "AAdHP correction".
Subsequently, both the previously mentioned schemes have been also applied for the numerical solution of SLPs with general boundary conditions. In this case, a suitable approximation of the first order derivative of the eigenfunction, occurring in at least one extreme of the interval of integration, enters into the discrete problem. In addition, in [3] Anderssen and de Hoog studied the effectiveness of the asymptotic correction in improving the accuracy of the numerical eigenvalues provided by the three-point scheme. A similar approach has been conducted for the Numerov method by Andrew in [5, 6].

Recently, in [1] a family of Boundary Value Methods (BVMs) has been introduced for the approximation of the eigenvalues of SLPs with Dirichlet boundary conditions which has provided positive results with respect to the corrected Numerov method. The aim of this paper is the extension of such methods for the eigenvalue estimates of the SLP (1)-(2). The Forward and Backward Differentiation Formulas, with the same order of accuracy of the applied BVM, are used for discretizing $y'(0)$ and $y'(\pi)$, respectively. The resulting discrete problem is a generalized matrix eigenvalue one and a compact formulation of it is given which includes all possible types of boundary conditions. Moreover, the band structure of the involved matrices is preserved while the same does not happen for the Numerov method if the SLP is subject to (2) with $|a_1a_2| + |b_1b_2| \neq 0$ (see [5] for further details).
An analysis of the error in the approximation of the kth eigenvalue provided by the proposed schemes is reported showing that, for a BVM of order p, if q is "sufficiently" regular as we always assume hereafter, its asymptotic behaviour is $O(k^{p+1}h^{p-\frac{1}{2}}) + O(k^{p+2}h^p)$, i.e. the same derived in [1]. Consequently, the new methods turn out to be competitive with respect to the corrected Numerov method at least for the lowest index eigenvalues. In addition, there is numerical evidence that the asymptotic correction extends the string of eigenvalues for which such competitiveness persists.

The paper is organized as follows: in Section 2 a survey of the two classical discretization methods and of the corresponding asymptotic correction technique is reported; in Section 3 the mentioned BVMs together with the discretization of the boundary conditions (2) are described; Section 4 deals with the analysis of the error in the eigenvalue estimates provided by the new methods; Section 5 briefly discusses a version of the same schemes defined over an assigned nonuniform mesh. Finally, in Section 6, some numerical results showing the possible advantages that may arise from the use of the proposed methods are reported.

2 Three-point scheme and Numerov's method

The three-point scheme and the Numerov method are designed for the direct approximation of the solution of a second order differential equation of special type

$$y'' = f(x, y)\,,\ x \in [0, \pi]\,, \tag{4}$$

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

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

a uniform mesh over the time integration interval, with y_n the numerical approximation of $y(x_n)$ and with $f_n = f(x_n, y_n)$, the three-point scheme discretizes (4) as

$$\frac{y_{n-1} - 2y_n + y_{n+1}}{h^2} = f_n, \quad n = 1, 2, \ldots, N, \tag{5}$$

while the Numerov method is

$$\frac{y_{n-1} - 2y_n + y_{n+1}}{h^2} = \frac{1}{12}(f_{n-1} + 10f_n + f_{n+1}), \quad n = 1, 2, \ldots, N. \tag{6}$$

As it is well known, the order of accuracy is $p = 2$ for the former method and $p = 4$ for the latter one.
When applied to (1), both (5) and (6) can be written in matrix form as

$$M_h \tilde{\mathbf{y}}^{(h)} \equiv \left(-\frac{1}{h^2}\tilde{T} + \tilde{B}\tilde{Q} \right) \tilde{\mathbf{y}}^{(h)} = \lambda^{(h)} \tilde{B} \tilde{\mathbf{y}}^{(h)}\,, \tag{7}$$

where $\lambda^{(h)}$ represents the approximation of one of the exact eigenvalues, $\tilde{\mathbf{y}}^{(h)} = (y_0, y_1, \ldots, y_{N+1})^T$ and, by denoting with J the anti-identity matrix of size N, with $\mathbf{e}_1^{(N)}$ the first unit vector in $\mathbb{R}^N$ and by posing $q_i = q(x_i)$ for each i, the matrices $\tilde{T}$ and $\tilde{Q}$ are given by

$$\tilde{T} = \left(\mathbf{e}_1^{(N)} \mid T \mid J\mathbf{e}_1^{(N)} \right) = \left(\begin{array}{c|ccccc|c} 1 & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & 1 & -2 & 1 & \\ & & & & 1 & -2 & 1 \end{array} \right) \in \mathbb{R}^{N \times (N+2)}\,, \tag{8}$$

$$\tilde{Q} = \begin{pmatrix} q_0 & & \\ & Q & \\ & & q_{N+1} \end{pmatrix}\,, \qquad Q = \operatorname{diag}(q_1, \ldots, q_N)\,.$$

Finally, the matrix $\tilde{B}$ is defined as

$$\tilde{B} = (\boldsymbol{\beta}_0 \mid B \mid J\boldsymbol{\beta}_0) \in \mathbb{R}^{N \times (N+2)}\,, \quad \boldsymbol{\beta}_0 \in \mathbb{R}^N\,,$$

with $\boldsymbol{\beta}_0 = \mathbf{0}$, the zero vector in $\mathbb{R}^N$, and $B = I$, the identity matrix, for the three-point scheme while $\boldsymbol{\beta}_0 = \frac{1}{12}\mathbf{e}_1^{(N)}$ and $B = I + \frac{1}{12}T$ for the Numerov method.
Concerning the boundary conditions they are handled differently depending on whether they are of Dirichlet type or not. In particular, for the condition imposed at $x = 0$:

- if $a_2 = 0$ (i.e. $y(0) = 0$) then in (7) the first entry in $\tilde{\mathbf{y}}^{(h)}$ and the first column in M_h and in $\tilde{B}$ are simply deleted;

- if $a_2 \neq 0$ then one equation obtained by combining a sufficiently accurate approximation of $y'(0)$ with (5) or (6), used with $n = 0$, is added to (7) (see [3, 5] for further details).

The boundary condition at $x = \pi$ is handled similarly.
Altogether these two schemes replace the continuous problem with a matrix eigenvalue one. For example, in the simplest case of the Dirichlet boundary conditions (3), this is given by

$$\left(-\frac{1}{h^2}T + BQ\right)\mathbf{y}^{(h)} = \lambda^{(h)}B\mathbf{y}^{(h)}, \tag{9}$$

with

$$\mathbf{y}^{(h)} = (y_1, \ldots, y_N)^T . \tag{10}$$

More generally, independently of the type of boundary conditions, the three-point scheme (5) generates a classical eigenvalue problem for a tridiagonal matrix [3].
The Numerov method (6), instead, provides a generalized eigenvalue problem with tridiagonal coefficient matrices in the case of SLPs with natural boundary conditions, that is one among (3) and

$$y'(0) = y'(\pi) = 0\,, \tag{11}$$
$$y(0) = y'(\pi) = 0\,, \tag{12}$$
$$y'(0) = y(\pi) = 0\,, \tag{13}$$

while a nonlinear dependence of $\lambda^{(h)}$ occurs in the discrete problem if the coefficients in (2) are such that $|a_1a_2| + |b_1b_2| \neq 0$, [4]. In the latter case, a further handling of the discrete problem with the goal of removing the nonlinearity thus getting again a generalized eigenvalue problem has been introduced by Andrew in [5]. It has to be noted, however, that the proposed technique has two important side effects. The first one is constituted by the fact that the new discrete problem no longer involves only banded matrices. The second effect is the production of spurious numerical eigenvalues which the author suggests should not be difficult to identify since they are characterised by a much greater magnitude than the true ones. A rigorous proof of this assertion, however, is currently not available.
It is known that the two methods (5) and (6) give results with $O(k^{p+2}h^p)$ error in the computed estimate of the eigenvalues. In order to reduce the growth in the error with increasing k, the asymptotic correction technique is frequently applied successfully. This method involves the computation of the improved estimate $\tilde{\lambda}_k^{(h)}$ for λ_k as

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

where Λ_k and $\Lambda_k^{(h)}$ represent the kth exact and numerical eigenvalue for $q \equiv 0$, respectively. The basic argument that has led to the development of this technique is the observation that for both schemes the error $\lambda_k - \lambda_k^{(h)}$ is essentially independent of the potential q. Moreover, for SLPs subject to (3), (11)-(13) or to

$$y'(0) = Cy(0), \quad y'(\pi) = Cy(\pi)\,, \qquad C \neq 0,$$

the error $\Lambda_k - \Lambda_k^{(h)}$ is known in closed form so that the asymptotic correction can be applied at negligible extra cost. For the remaining types of boundary conditions the eigenvalues Λ_k and $\Lambda_k^{(h)}$ are attainable as the limit of suitable numerical sequences [3, 5, 6]. When kh is "sufficiently" small, the error presented in the corrected eigenvalues $\tilde{\lambda}_k^{(h)}$ is shown to be $O(h^2)$ for the three-point scheme independently of the values of a_1, a_2, b_1, and b_2 in (2), [3]. For the Numerov method, instead, this error is $O(k^3h^4)$; this is proved in [7] for SLPs with Dirichlet boundary conditions (3) while, at least to the best of our knowledge, it is only conjectured on the basis of numerical results for the other types of boundary conditions [4, 5].

3 Boundary Value Methods

In [1] a family of BVMs has been introduced for the numerical approximation of the eigenvalues of regular SLPs subject to the Dirichlet boundary condition (3). We recall that BVMs are composed of Linear Multistep Formulas (LMF's) combined in a suitable way, [8]. More precisely, a so-called *main formula* is coupled with a set of *additional* ones. In particular, when applied to (4), the (2ν)-step ($\nu \geq 1$) main formula of the BVMs considered in [1] reads

$$\frac{y_{n-1} - 2y_n + y_{n+1}}{h^2} = \sum_{i=0}^{2\nu} \beta_i^{(\nu,2\nu)} f_{n+i-\nu}, \qquad n = \nu, \nu+1, \ldots, N+1-\nu. \tag{14}$$

By setting $\nu = 1$, the three-point scheme and the Numerov method are obtained with an appropriate choice of the coefficients $\beta_i^{(1,2)}$, so that such two methods represent particular instances of (14).
When $\nu > 1$ the main formula is used with the following two sets of additional ones

$$\frac{y_{s-1} - 2y_s + y_{s+1}}{h^2} = \sum_{i=0}^{2\nu} \beta_i^{(s,2\nu)} f_i\,, \qquad s = 1, 2, \ldots, \nu-1, \tag{15}$$

$$\frac{y_{m-1} - 2y_m + y_{m+1}}{h^2} = \sum_{i=0}^{2\nu} \beta_i^{(s,2\nu)} f_{m-s+i}, \quad s = \nu+1, \ldots, 2\nu-1, \quad m = N+1+s-2\nu, \tag{16}$$

called the *initial* and the *final* methods, respectively.
For each $s = 1, 2, \ldots, 2\nu-1$, the coefficients $\beta_i^{(s,2\nu)}$ are uniquely determined by imposing the sth formula to have the highest attainable order of accuracy given by $2\nu+1$. As proved in [1], the so-obtained composite scheme (14)-(16) turns out to be symmetric, namely $\beta_i^{(s,2\nu)} = \beta_{2\nu-i}^{(2\nu-s,2\nu)}$, $i = 0, 1, \ldots, 2\nu$, $s = 1, 2, \ldots, \nu$. In particular, the main formula, which is the one corresponding to $s = \nu$, is a symmetric LMF and this implies that its order of accuracy is actually $p = 2\nu+2$ since it must be even and not less than $2\nu+1$ by construction. In the sequel, when speaking about the order of the composite scheme (14)-(16) we will refer to the order p of its main formula. It has to be noted that in this setting the case $\nu = 1$ corresponds to the Numerov method and not to the three-point scheme.

The described (2ν)-step BVM applied to (1) gives the system of equations (7) via the formal substitution

$$\tilde{B} \qquad \rightarrow \qquad \tilde{B}^{(\nu)} = \left(\boldsymbol{\beta}_0^{(\nu)} | B^{(\nu)} | J\boldsymbol{\beta}_0^{(\nu)}\right) \tag{17}$$

where, by omitting for simplicity the second upper index for the coefficients β,

$$\boldsymbol{\beta}_0^{(\nu)} = \left(\beta_0^{(1)}, \beta_0^{(2)}, \ldots, \beta_0^{(\nu)}, 0, \ldots, 0\right)^T \in \mathbb{R}^N\,,$$

ν	η_ν	α_0	α_1	α_2	α_3	α_4	α_5	α_6	α_7
2	60	-12	-65	120	-60	20	-3		
3	420	-60	-609	1260	-1050	700	-315	84	-10

Table 1: Coefficients of the $(2\nu+2)$-step Forward Differentiation Formula with $\nu = 2, 3$.

$$B^{(\nu)} = \begin{pmatrix} \beta_1^{(1)} & \cdots & \beta_\nu^{(1)} & \cdots & \beta_{2\nu-1}^{(1)} & \beta_{2\nu}^{(1)} & & & \\ \vdots & & \vdots & & \vdots & \vdots & & & \\ \beta_1^{(\nu-1)} & \cdots & \beta_\nu^{(\nu-1)} & \cdots & \beta_{2\nu-1}^{(\nu-1)} & \beta_{2\nu}^{(\nu-1)} & & & \\ \beta_1^{(\nu)} & \cdots & \beta_\nu^{(\nu)} & \cdots & \beta_1^{(\nu)} & \beta_0^{(\nu)} & & & \\ \beta_0^{(\nu)} & \beta_1^{(\nu)} & \cdots & \beta_\nu^{(\nu)} & \cdots & \beta_1^{(\nu)} & \beta_0^{(\nu)} & & \\ & \ddots & \ddots & & \ddots & & \ddots & \ddots & \\ & & \beta_0^{(\nu)} & \beta_1^{(\nu)} & \cdots & \beta_\nu^{(\nu)} & \cdots & \beta_1^{(\nu)} & \beta_0^{(\nu)} \\ & & & \beta_0^{(\nu)} & \beta_1^{(\nu)} & \cdots & \beta_\nu^{(\nu)} & \cdots & \beta_1^{(\nu)} \\ & & & \beta_{2\nu}^{(\nu-1)} & \beta_{2\nu-1}^{(\nu-1)} & \cdots & \beta_\nu^{(\nu-1)} & \cdots & \beta_1^{(\nu-1)} \\ & & & \vdots & \vdots & & \vdots & & \vdots \\ & & & \beta_{2\nu}^{(1)} & \beta_{2\nu-1}^{(1)} & \cdots & \beta_\nu^{(1)} & \cdots & \beta_1^{(1)} \end{pmatrix}_{N\times N} . \quad (18)$$

Let us now discuss the discretization of the boundary conditions (2) we have considered. The first one of them is approximated by applying the $(2\nu+2)$-step Forward Differentiation Formula (FDF) given by

$$\sum_{i=0}^{2\nu+2} \alpha_i y(x_i) = hy'(0) + \tau_L \quad (19)$$

where $\{\alpha_i\}_{i=0}^{2\nu+2}$ are the coefficients of the formula uniquely determined by imposing the associated local truncation error τ_L to be $O(h^{2\nu+3})$. As examples, in Table 1 the coefficients of the FDF with $\nu = 2, 3$, multiplied by the corresponding factor η_ν, have been reported.
From the previous equation, by neglecting τ_L, the following approximation of the first boundary condition is therefore obtained

$$a_2 \sum_{i=0}^{2\nu+2} \alpha_i y_i = ha_1 y_0 \, . \quad (20)$$

Clearly, this can be equivalently written as

$$y_0 = \frac{a_2}{ha_1 - a_2\alpha_0} \sum_{i=1}^{2\nu+2} \alpha_i y_i = \gamma_L \boldsymbol{\alpha}^T \mathbf{y}^{(h)}, \quad (21)$$

where $\mathbf{y}^{(h)}$ is given in (10),

$$\gamma_L = \frac{a_2}{ha_1 - a_2\alpha_0} \qquad \text{and} \qquad \boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_{2\nu+2}, 0, \ldots, 0)^T \in \mathbb{R}^N. \quad (22)$$

The boundary condition at the right endpoint is discretized similarly by using the $(2\nu+2)$-step Backward Differentiation Formula (BDF) of order $2\nu+2$ thus getting

$$b_2 \sum_{i=0}^{2\nu+2} \hat{\alpha}_i y_{N-1-2\nu+i} = hb_1 y_{N+1} \, . \quad (23)$$

The coefficients of the FDF and the BDF with the same stepnumber satisfy $\alpha_j = -\hat{\alpha}_{2\nu+2-j}$, $j = 0, 1, \ldots, 2\nu+2$. In vector notation, (23) therefore becomes

$$y_{N+1} = -\gamma_R(\boldsymbol{\alpha}^T J)\mathbf{y}^{(h)} \tag{24}$$

where, we recall, J denotes the anti-identity matrix of size N and

$$\gamma_R = \frac{b_2}{hb_1 + b_2\alpha_0}\,. \tag{25}$$

Now, combining (7), (17) with (21) and (24), after some computation one obtains

$$M\mathbf{y}^{(h)} = \lambda^{(h)} S\mathbf{y}^{(h)}, \tag{26}$$

where

$$M = -\frac{1}{h^2}T + B^{(\nu)}Q + \gamma_L\left(-\frac{1}{h^2}\mathbf{e}_1^{(N)} + q_0\boldsymbol{\beta}_0^{(\nu)}\right)\boldsymbol{\alpha}^T - \gamma_R J\left(-\frac{1}{h^2}\mathbf{e}_1^{(N)} + q_{N+1}\boldsymbol{\beta}_0^{(\nu)}\right)\boldsymbol{\alpha}^T J \tag{27}$$

and

$$S = B^{(\nu)} + \gamma_L\boldsymbol{\beta}_0^{(\nu)}\boldsymbol{\alpha}^T - \gamma_R J\boldsymbol{\beta}_0^{(\nu)}\boldsymbol{\alpha}^T J. \tag{28}$$

The equation (26) is the generalized eigenvalue problem that the considered BVM generates when applied for the approximation of the eigenvalues of the SLP (1)-(2). We want to emphasize the fact that every regular SLP subject to any possible type of boundary conditions leads to the discrete problem (26). In particular, for the latter conditions, it is sufficient to change the values of the coefficients γ_L and γ_R in (27) and (28) according to the assigned values of a_1, a_2, b_1, and b_2 in (2). For example, in the case of the Dirichlet boundary condition (3) it turns out that $\gamma_L = \gamma_R = 0$ so that (26) reduces to (9), again via the formal substitution (17).

4 Convergence analysis for the eigenvalue estimates

As usual, the analysis of the error in the eigenvalue approximations is based on the study of the local truncation error associated with the formula used. This is given by

$$\boldsymbol{\tau}_k = M\mathbf{y}_k - \lambda_k S\mathbf{y}_k,$$

where λ_k is the exact eigenvalue of index k while the entries of $\mathbf{y}_k$ are the projections of the corresponding eigenfunction, normalized to be of unit uniform norm, over the internal mesh points. By considering the derivation of the generalized eigenvalue problem (26), one can verify that

$$\boldsymbol{\tau}_k = \tilde{\boldsymbol{\tau}}_k + \gamma_L\left(-\frac{1}{h^2}\mathbf{e}_1^{(N)} + (q(0) - \lambda_k)\boldsymbol{\beta}_0^{(\nu)}\right)\tau_{k,L} + \gamma_R J\left(-\frac{1}{h^2}\mathbf{e}_1^{(N)} + (q(\pi) - \lambda_k)\boldsymbol{\beta}_0^{(\nu)}\right)\tau_{k,R}$$

where, see (19), $\tau_{k,L}$ is the local truncation error corresponding to the FDF that is used, $\tau_{k,R}$ is the same for the BDF that is used, while $\tilde{\boldsymbol{\tau}}_k$ is the one corresponding to the composite scheme (14)-(16). In particular, from the theory of LMFs follows that

$$\tau_{k,L} = \theta_L h^{p+1} y_k^{(p+1)}(\zeta_L), \qquad \tau_{k,R} = \theta_R h^{p+1} y_k^{(p+1)}(\zeta_R),$$

and that the entries of $\tilde{\boldsymbol{\tau}}_k$ are given by

$$\left(\tilde{\boldsymbol{\tau}}_k\right)_j = \begin{cases} \theta_\nu\, h^p y_k^{(p+2)}(\zeta_j), & j = \nu, \nu+1, \ldots, N+1-\nu, \\ \theta_j\, h^{p-1} y_k^{(p+1)}(\zeta_j), & \text{otherwise}, \end{cases}$$

where the θ-s are the principal error coefficients of the corresponding formula. As a consequence, if kh is "sufficiently" small and $\nu > 1$, the leading term in the entries of $\boldsymbol{\tau}_k$ has the following asymptotic behaviour [9]

$$(\boldsymbol{\tau}_k)_j = \begin{cases} O(h^p k^{p+2}) & j = \nu, \ldots, N-\nu, \\ O(h^{p-1} k^{p+1}), & \text{otherwise.} \end{cases} \tag{29}$$

The aim of the following result is to establish a relation between $\boldsymbol{\tau}_k$ and the error in the approximation of the kth eigenvalue. In the formulation of it we have assumed that S is invertible and this hypothesis will be maintained also in the sequel.

Theorem 4.1 *Let us assume that the matrix $Z = S^{-1}M$ is diagonalizable and let V_h be the corresponding matrix of eigenvectors normalized to be of unit length. Let λ_k, $\mathbf{y}_k$ and $\boldsymbol{\tau}_k$ be as above. Then*

$$\left|\lambda_k - \lambda_k^{(h)}\right| = \inf_{\mu \in \sigma(Z)} |\lambda_k - \mu| \leq \frac{\mathrm{cond}(V_h)\ \left\|S^{-1}\right\|\ \|\boldsymbol{\tau}_k\|}{\|\mathbf{y}_k\|}\,, \tag{30}$$

where $\sigma(Z)$ denotes the spectrum of Z and $\mathrm{cond}(V_h)$ is the condition number of V_h.

Proof. Similar to the one given for [2, Theorem 2.7] since the matrix S does not depend on the potential q. □

We observe that the assumption made on Z in the previous theorem seems to be reasonable since the SLP has simple eigenvalues and Z is a consistent discretization of the continuous problem.
The immediate consequence of (30) is the fact that in the case where $\mathrm{cond}(V_h)$ and $\left\|S^{-1}\right\|$ are bounded independently of N, the error in the estimate of the kth eigenvalue does have the same asymptotic behaviour as $\boldsymbol{\tau}_k$. For the schemes proposed here, it is not simple to derive theoretical results concerning the conditioning of V_h. Nevertheless, we conjecture the existence of an upper bound for $\mathrm{cond}(V_h)$ by virtue of the results of several numerical experiments we have carried out using the Euclidean norm. As an example, in Figure 1 we report the condition number of V_h for the 6-step BVM of order $p = 8$ applied to the SLPs defined by equation (1) with $q(x) = (0.1+x)^{-2}$ and boundary conditions of different types.

In order to study the behaviour of $\|S^{-1}\|_2$ with respect to N, some remarks about the structure of S are necessary. As proved in [1], the matrix $B^{(\nu)}$ in (18) can be decomposed as

$$B^{(\nu)} = p_\nu(T) + E_0^{(\nu)}\,, \qquad p_\nu(T) = I + \sum_{j=1}^{\nu} \omega_j T^j\,, \tag{31}$$

where T is defined in (8) and ω_j is the principal coefficient of the local truncation error for the $(2j)$-step main formula. 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. Thus, see (28),

$$S = p_\nu(T) + E_0^{(\nu)} + \gamma_L \boldsymbol{\beta}_0^{(\nu)} \boldsymbol{\alpha}^T - \gamma_R J \boldsymbol{\beta}_0^{(\nu)} \boldsymbol{\alpha}^T J \equiv p_\nu(T) + E_\nu,$$

where E_ν has a structure similar to that of $E_0^{(\nu)}$ with the difference that the two blocks not equal to zero have at most size $\nu \times (2\nu+2)$ and its entries depend on N (i.e., on h) when $|a_1 a_2| + |b_1 b_2| \neq 0$ due to the presence of the parameters γ_L and/or γ_R, see (22) and (25).
However, we observe that

$$\bar{\gamma}_L \equiv \lim_{h\to 0} \gamma_L = \begin{cases} -\frac{1}{\alpha_0} & \text{if } a_2 \neq 0 \\ 0 & \text{otherwise} \end{cases}\,, \qquad \bar{\gamma}_R \equiv \lim_{h\to 0} \gamma_R = \begin{cases} \frac{1}{\alpha_0} & \text{if } b_2 \neq 0 \\ 0 & \text{otherwise} \end{cases}\,.$$

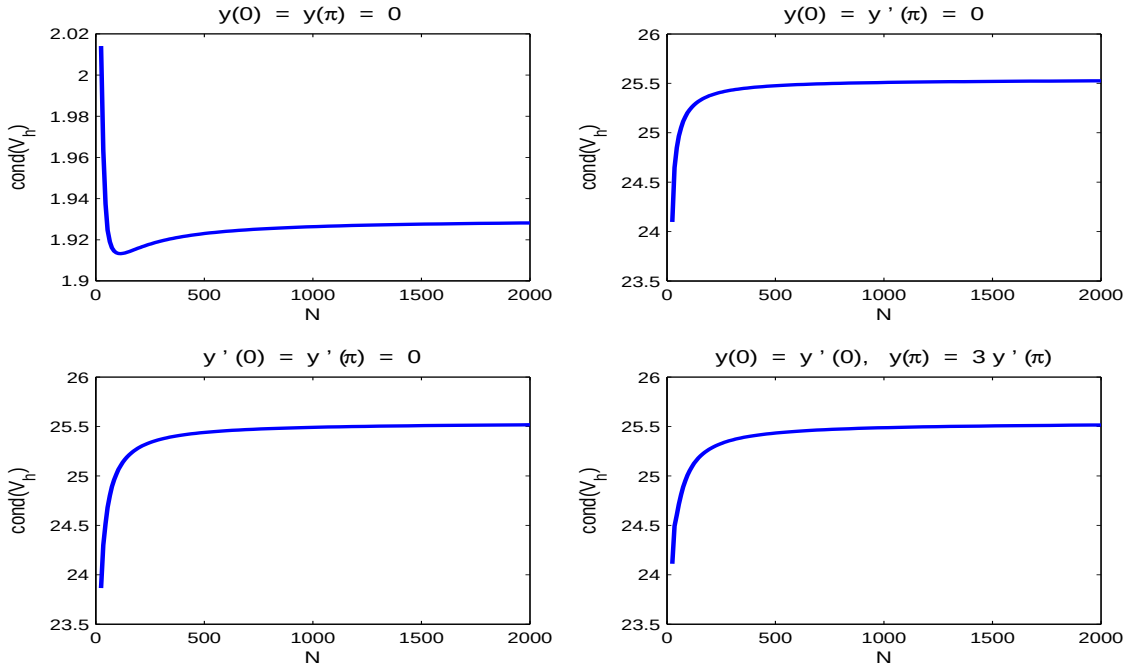

Figure 1: Cond(V_h) for some boundary conditions and $q(x) = (0.1 + x)^{-2}$.

Therefore, by denoting with

$$\bar{E}_\nu = E_0^{(\nu)} + \bar{\gamma}_L \boldsymbol{\beta}_0^{(\nu)} \boldsymbol{\alpha}^T - \bar{\gamma}_R J \boldsymbol{\beta}_0^{(\nu)} \boldsymbol{\alpha}^T J, \tag{32}$$

we can write

$$\begin{aligned} E_\nu &= \bar{E}_\nu + \Delta E_\nu(h)\,, \qquad \text{with} \qquad \lim_{h\to 0} \|\Delta E_\nu(h)\| = 0\,, \\ S &= p_\nu(T) + \bar{E}_\nu + \Delta E_\nu(h) \equiv \bar{S} + \Delta E_\nu(h)\,. \end{aligned} \tag{33}$$

The matrix $\bar{E}_\nu$ has the same structure of E_ν but its entries no longer depend on h. By considering that $S^{-1} = \left(I + \bar{S}^{-1}\Delta E_\nu(h)\right)^{-1} \bar{S}^{-1}$, one deduces that a sufficient condition for $\|S^{-1}\|_2$ to be bounded with respect to N is that the same holds true for $\|\bar{S}^{-1}\|_2$. The following result, similar to [1, Lemma 4.3], is stated here for proving that the latter property is verified at least for the (2ν)-step BVM with $\nu \leq 4$.

Lemma 4.2 *Let T be the tridiagonal matrix given in (8), $\bar{S}$ the coefficient matrix defined in (33) for the (2ν)-step BVM and $p_\nu(T)$ as in (31). Moreover, let*

$$F_\nu = p_\nu(T)(\bar{E}_\nu)^T + \bar{E}_\nu p_\nu(T) + \bar{E}_\nu(\bar{E}_\nu)^T,$$

see (32), 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 $N \geq 6\nu + 4$

(*i*) $\mu_1(F_\nu)$ *is independent of* N;

(*ii*) $\hat{\mu}_\nu \leq \mu_1(p_\nu^2(T))$ *for each* N;

(*iii*) *if* $\hat{\mu}_\nu + \mu_1(F_\nu) > 0$ *then* $\|\bar{S}^{-1}\|_2 \leq (\hat{\mu}_\nu + \mu_1(F_\nu))^{-\frac{1}{2}} \equiv \delta_\nu$.

The numerical computed values of $\mu_1(F_\nu)$ and δ_ν for SLPs subject to the Dirichlet boundary conditions (3) have already been reported in [1, Table 2]. For the remaining types of boundary conditions (11)-(13), by direct inspection we find that the values of $\mu_1(F_\nu)$ coincide and at least for $\nu = 1, 2, 3, 4$ they satisfy the hypothesis in the third statement of the previous lemma. In Table 2 such values of $\mu_1(F_\nu)$ and the relative bound δ_ν for $\|\bar{S}^{-1}\|_2$ have been listed.

ν	$\hat{\mu}_\nu$	$\mu_1(F_\nu)$	δ_ν
1	0.4444	−0.0251	1.5444
2	0.3600	−0.0918	1.9310
3	0.3217	−0.2107	3.0015
4	0.2990	−0.2933	13.2320

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

The following theorem completes the convergence analysis for the BVMs described in the previous section applied for approximating the eigenvalues of the SLP (1)-(2). By virtue of (29), its proof is analogous to that given for [1, Theorem 4.4].

Theorem 4.3 *Let* λ_k *be the* k*th exact eigenvalue of the SLP (1)-(2) and* $\lambda_k^{(h)}$ *be the corresponding numerical eigenvalue provided by the* (2ν)*-step BVM (14)-(16), eventually coupled with (20) and/or (23). Moreover, let* V_h *be the matrix of eigenvectors normalized to be of unit length of the matrix* $S^{-1}M$*. Then, if* $\nu > 1$, $\mathrm{cond}(V_h)$ *and* $\|S^{-1}\|$ *are bounded independently of* N *in Euclidean norm and if* kh *is "sufficiently" small, one has*

$$|\lambda_k - \lambda_k^{(h)}| \sim O(k^{p+1}h^{p-\frac{1}{2}}) + O(k^{p+2}h^p)\,, \qquad p = 2\nu + 2\,.$$

5 BVMs with variable stepsize

The numerical experiments we have conducted with the methods described in Section 3 show the presence of complex eigenvalues in the spectrum of the matrix pencil (M, S). As already observed in [1], this drawback appears when the order p of the applied BVM increases and it seems to be limited to at most two couples of complex conjugate pairs. Anyway, it is in contrast with the peculiarity of a regular SLP with a real-valued potential q of having a real spectrum.
The cause of this incongruity is the presence of the auxiliary methods (15)-(16) and the discretization of the boundary conditions via the use of the FDF and/or BDF methods.
A possible strategy for reducing such an effect consists in taking a finer mesh near the extremes of the interval of integration, namely, the interval $[0, \pi]$ is discretized as follows:

$$x_0 = 0\,, \quad x_i = x_{i-1} + h_i\,, \quad i = 1, 2, \ldots, N+1\,, \quad x_{N+1} = \pi\,, \tag{34}$$

where

$$\begin{cases} h_1 \leq h_2 \leq \cdots \leq h_\eta\,, & \\ h_i = h_\eta\,, & i = \eta+1, \ldots, N-\eta+1\,, \\ h_i = h_{N-i+2}\,, & i = N-\eta+2, \ldots, N+1. \end{cases} \tag{35}$$

The choice of the nonuniformly distributed nodes can be made in several ways. For example, they can be derived starting from the zeros of suitable orthogonal polynomials of degree $2\eta+1$, as done in [1], or arranged with a geometric progression distribution which, for $\eta > 1$, is given by

$$h_i = \xi^{\eta-i}\,\frac{\pi}{N-2\eta+5}, \quad i = 1,2,\ldots,\eta, \qquad \text{with} \quad \xi \in (0,1), \quad \sum_{i=1}^{\eta-1}\xi^i = 1, \tag{36}$$

see [8, pg. 284] for further details.
The LMFs occurring in the discretization of the continuous problem over the nonuniform mesh are obtained similarly with respect to (14)-(16), (20) and (23). This leads to a generalized eigenvalue problem

$$M_V \mathbf{y}^{(h_\eta)} = \lambda^{(h_\eta)} S_V \mathbf{y}^{(h_\eta)},$$

where M_V and S_V are the analogs of the matrices M and S given in (27) and (28), respectively, and S_V is assumed to be invertible.
The results of some experiments suggest that, for the nonuniform mesh (34)-(36), the best performances of the methods are obtained by setting $\eta = \nu + 1$. Moreover, for such values of η complex eigenvalues no longer belong to the numerical spectrum.
Concerning the analysis of convergence of the so-obtained approximations $\lambda_k^{(h_\eta)}$ 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 $\|S_V^{-1}\|$ is bounded as well. These properties of M_V and S_V are confirmed by the results of the numerical experiments we have done with several potentials q.
Under these assumptions, arguments analogous to those used in Section 4 allow us to prove that

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

6 Numerical examples

The matrix methods introduced in Sections 3 and 5 have been applied to some SLPs (1)-(2) with classical potentials and their performances have been compared with that of the corrected Numerov method used as described in [5].
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, [10]. The reported comparisons are all based on the number N of mesh points alone. A deeper comparison with Numerov's method should take into account the different structure of the matrices involved in the generalized eigenvalue problem. In particular, in the case of SLPs subject to one of the natural boundary conditions given in (3), (11)-(13) the matrices M and S in (27)-(28) corresponding to the higher order methods have a larger bandwidth with respect to the analogs of Numerov's method which are tridiagonal. This leads to an increase of the computational cost whose exact quantification is however rather difficult since it is strictly related to the routine of linear algebra used and to the optimizations therein introduced.

Example 1. Let us consider the Coffey-Evans equation [12] having $q(x) = 40\cos(2x) + (20\sin(2x))^2$ subject to Neumann boundary conditions given by

$$y'(0) = 0\,, \qquad y'(\pi) = 0\,.$$

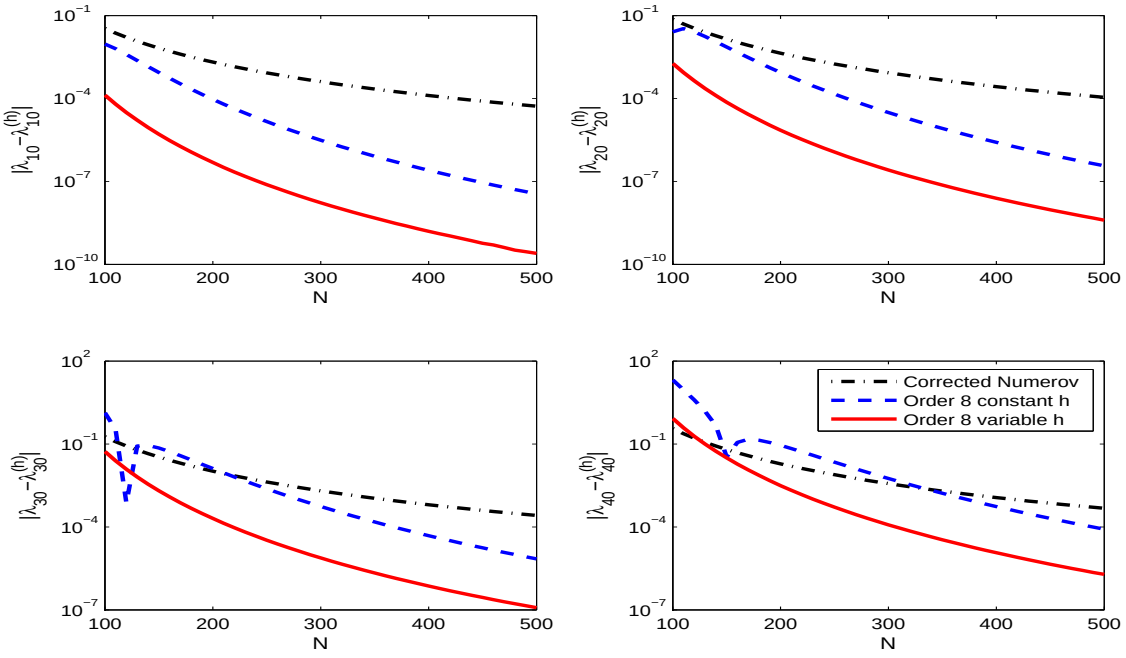

Figure 2: Numerical results for the SLP in Example 1 provided by the corrected Numerov method (dash-dotted line), the BVM of order 8 with constant (dashed line) and variable (solid line) stepsize.

The methods applied for the approximation of its eigenvalues are the 6-step BVM of order 8 both with constant and variable (geometrically distributed, see (36)) stepsize and the corrected Numerov method. For this problem, in fact, the asymptotic correction for the latter method can be applied with a negligible extra cost. In Figure 2, the corresponding errors $\left|\lambda_k - \lambda_k^{(h)}\right|$ with $k = 10, 20, 30, 40$ for increasing values of N (i.e. for $h \to 0$) have been reported.
As one can see, the proposed schemes turn out to be competitive with respect to the corrected Numerov method even without the application of any kind of a posteriori correction. Moreover, the results provided by the BVM with nonuniform mesh are considerably more accurate than those given by the same method with uniform mesh. A possible explanation of this behaviour lies in the fact that the refinement of the mesh near the extremes of the interval of integration leads the FDF and BDF methods to provide better discretizations of the boundary conditions. For this reason, in the sequel, we will consider only the BVMs defined over a nonuniform mesh.
Finally, it is worth mentioning that for this and the following examples, the proposed schemes with an appropriate order of accuracy and, eventually, with the application of the asymptotic correction technique turn out to be competitive also with respect to the corrected Numerov method improved with one extrapolation.

Example 2. Let us consider the SLP with potential $q(x) = (0.1+x)^{-2}$ and boundary conditions

$$y(0) = 3y'(0), \qquad y(\pi) = -2y'(\pi)\,.$$

In this case we have applied the uncorrected and the corrected BVM of order 8 with variable (geometrically distributed) stepsize. The results obtained together with those given by the corrected Numerov method have been reported in Figure 3 where a notation similar to the one adopted in the previous example has been used. From the first two subplots, one immediately deduces that the

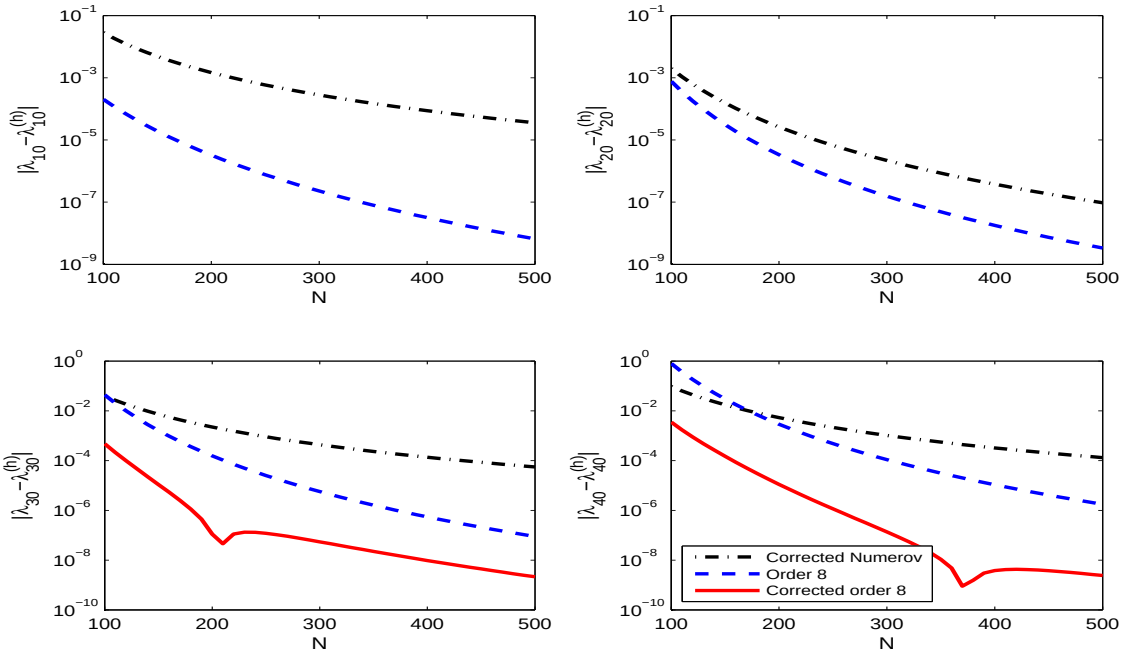

Figure 3: Numerical results for the SLP in Example 2 provided by the corrected Numerov method (dash-dotted line), the uncorrected (dashed line) and the corrected (solid line) BVM of order 8 with variable stepsize.

uncorrected BVM is competitive with respect to the corrected Numerov method in the case where the interest is focused in finding an accurate approximations of the first eigenvalues. Moreover, as shown in the last two subplots, the application of the asymptotic correction technique turns out to be successfull in improving the accuracy of the higher index eigenvalues estimates that the former method provides. This fact allows us to extend the range of index of the eigenvalues for which such a scheme is competitive with respect to the corrected Numerov method. In addition, we have to recall that for the boundary conditions of the SLP considered in this example, the asymptotic correction for Numerov's method cannot be operated at negligible extra cost since the error for $q \equiv 0$ is not known in closed form (see [5]).

Example 3. Let us consider the SLP with potential $q(x) = 10\cos(2x)$ and boundary conditions

$$y(0) = 4y'(0), \qquad y(\pi) = 0\,.$$

Here the approximations of the eigenvalues have been computed by applying the corrected Numerov method and the corrected 4 and 6 step BVM of order 6 and 8, respectively, with variable (geometrically distributed) stepsize. The results obtained have been reported in Figure 4 and comments similar to the ones made in the previous example apply also in this case.

7 Conclusions

A family of BVMs has been introduced for the approximation of the eigenvalues of regular SLPs with general boundary conditions and a compact formulation of the corresponding discrete prob-

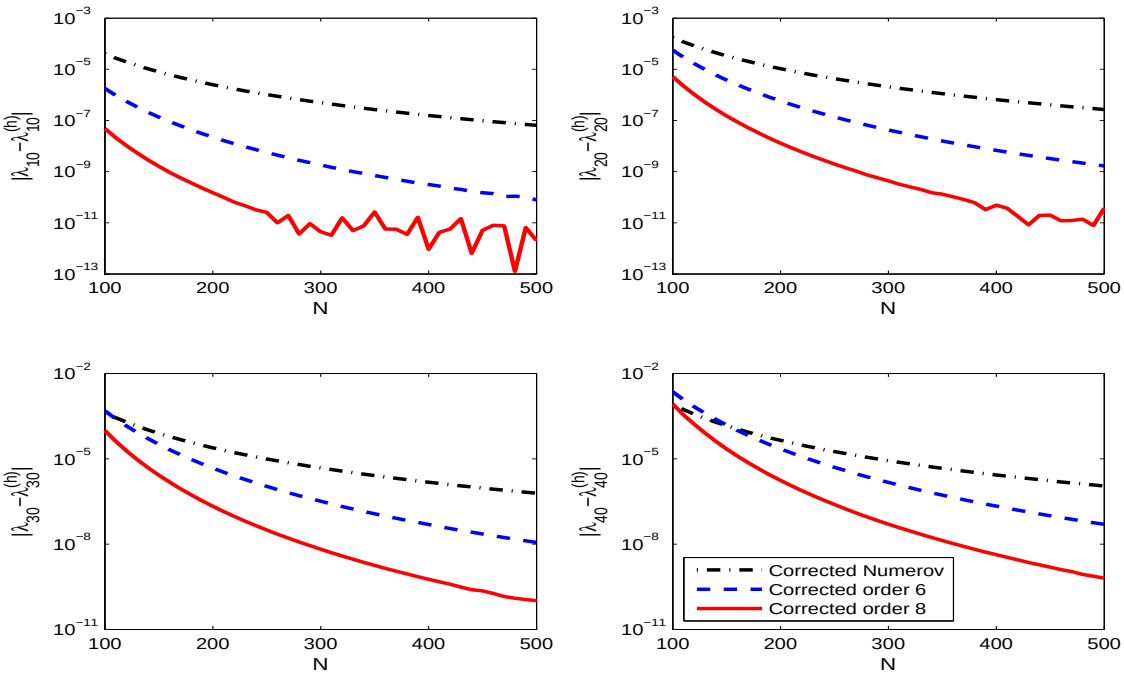

Figure 4: Numerical results for the SLP in Example 3 provided by the corrected Numerov method (dash-dotted line), the corrected variable stepsize BVMs of order 6 (dashed line) and 8 (solid line).

lems has been given. The numerical experiments we have carried out show an appreciable competitiveness of the proposed schemes, eventually after the application of the asymptotic correction, with respect to the corrected Numerov method.

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