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Exponentially-fitted Numerov methods

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Abstract

The error in the estimate of the kth eigenvalue of a regular Sturm–Liouville problem obtained by Numerov's method with mesh length h is $\mathcal{O}(k^6h^4)$. It is shown that the error can be reduced to $\mathcal{O}(k^3h^4)$ by using one of the three versions of the exponentially-fitted Numerov method. Numerical examples demonstrate the usefulness of this approach even for low values of k.

Keywords: Exponential fitting; Numerov methods; Eigenvalues

1. Introduction

For a long time there has been much interest in problems requiring the efficient and accurate computation of a large number of eigenvalues of regular Sturm–Liouville problems, which can be written without loss of generality as

$$-y'' + qy = \lambda y, \tag{1}$$

with boundary conditions of the type

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

Here $q(x)$ is the so-called potential function. When finite element or finite difference methods are used to approximate the eigenvalues $\lambda_1 < \lambda_2 < \lambda_3 < \cdots$ of (1) by the eigenvalues $\lambda_1^{(n)} < \lambda_2^{(n)} < \lambda_3^{(n)} < \cdots$ of an algebraic eigenvalue problem of order n, the error $|\lambda_k^{(n)} - \lambda_k|$, $(k = 1, 2, \ldots, n)$ is known to increase rapidly with k. Much recent efforts have been devoted to finding more uniformly valid approximations. Several computer codes have been developed by which very accurate high-lying eigenvalues can be obtained. As examples we can refer to the codes SLEIGN and SLEIGN2 [9], which are based on Prüfer's transformation with a fixed-scale factor, shooting and initial value codes, SLEDGE [12], which is using the coefficient approximation theory of Pruess, SLCPM12 [14], a FORTRAN90 package based on the CPM philosophy and MATSLISE [19], a MATLAB package based on higher order CPM methods. On the other side a correction error technique is developed starting with the paper of Paine, de Hoog and Anderssen [20], where it is

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shown in the case of the second order centered finite difference method with uniform mesh that the error, when q is a constant, has the same asymptotic form (i.e. for $k \to \infty$) as the error for general $q(x)$. They showed that the accuracy of the estimates obtained for high eigenvalues can be improved dramatically at negligible extra cost by using the known error for $q \equiv 0$ to correct the estimates for general $q(x)$. Andrew and Paine [7] have studied the error on the numerical eigenvalue $\Lambda_k^{(n)}$ related to Numerov's method and obtained the following result:

$$|\Lambda_k^{(n)} - \lambda_k| = \mathcal{O}(k^6 h^4). \tag{3}$$

By techniques analogous to the ones of Paine et al. they have proved that, when $q \in \mathbb{C}^4[0, \pi]$, there exists an α, independent of n, such that the corrected eigenvalues $\tilde{\Lambda}_k^{(n)}$, obtained by Numerov's method, satisfy

$$|\tilde{\Lambda}_k^{(n)} - \lambda_k| \leqslant c k^3 h^4, \quad 1 \leqslant k \leqslant \alpha n, \ \ \alpha < 1. \tag{4}$$

We like to remark that the result proved in [7] is in fact stronger than (4). In [7] it is proved that, for all $q \in \mathbb{C}^4[0, 1]$, there exists a number $c(q)$, depending only on q, such that, for all natural numbers n and $k = 1, \ldots, n$,

$$|\tilde{\Lambda}_k^{(n)} - \lambda_k| \leqslant c(q) k^4 h^5 / \sin(kh).$$

This implies that for *all* $\alpha \in (0, 1)$, a c in (4) may be found, and that c is given by the simple formula $c_0 \alpha\pi / \sin(\alpha\pi)$, where c_0 is independent of α. Andrew et al. have further developed a lot of analogous asymptotic correction theories for various finite difference and finite element methods [1–6,8]. Vanden Berghe and De Meyer [22] have developed particular linear multistep methods, especially Numerov type methods, with step-dependent coefficients for second-order differential equations of the type $y'' = f(x, y)$. These methods integrate exactly the functions $\sin(\omega x)$ and $\cos(\omega x)$. The parameter ω can be related to the period of the solution of (1). For the modified Numerov method in [22] it is proved that the numerical eigenvalues ${}^{(1)}\Sigma_k^{(n)}$ satisfy for all functions $q \in \mathbb{C}^4[0, \pi]$

$$|{}^{(1)}\Sigma_k^{(n)} - \lambda_k| \leqslant c^{(1)} k^3 h^4, \quad 1 \leqslant k \leqslant \alpha n, \ \ \alpha < 1. \tag{5}$$

This modified Numerov method constructed out of first principles belongs to the class of the so-called exponentially-fitted (EF) Numerov methods derived and discussed in several papers [10,13,15,16,21] and a book [17]. In this paper we shall investigate the two EF Numerov methods which have not yet been applied to Sturm–Liouville methods of the form (1). In Section 2, the different versions of the EF Numerov methods are introduced and the main properties are discussed. In Section 3, a theorem of the forms (4) and (5) is proved for those methods. In Section 4, the theoretical results of the theorem are demonstrated by means of numerical examples.

2. The EF Numerov methods

The EF Numerov methods have been discussed in the Appendix of [10] and in [17, pp. 192–198]. When applied to a second-order differential equation of the type $y'' = f(x, y)$ they all have the same form, i.e.

$$y_{n+1} + a_1 y_n + y_{n-1} = h^2 [b_0 (f_{n+1} + f_{n-1}) + b_1 f_n], \tag{6}$$

where y_n and f_n are short-hand notations for the numerical approximation of $y(x)$ and $f(x, y)$ in the point x_n, respectively. There exist one classical and three EF Numerov methods defined by the following values for the parameters a_1, b_0 and b_1 and the leading terms of the local truncation errors (we write down the expressions in terms of trigonometric functions and not in terms of exponential ones):

- S_0 (the classical scheme):

$$a_1 = -2, \quad b_0 = \frac{1}{12}, \quad b_1 = \frac{5}{6}, \quad lte_{S_0} = -\frac{h^6}{240} y^{(6)}(x_n).$$

- S_1, integrating exactly $1, x, x^2, x^3$ and the pair $\sin(\omega x), \cos(\omega x)$.

$$a_1 = -2, \quad b_0 = \frac{\theta^2 - 2(1-\cos(\theta))}{2\theta^2(1-\cos(\theta))}, \quad b_1 = 1 - 2b_0,$$

$$lte_{S_1} = -h^6 \frac{1-12b_0}{12\theta^2}(\omega^2 y^{(4)}(x_n) + y^{(6)}(x_n))$$

with $\theta = \omega h$.

- S_2, integrating exactly $1, x$ and the pairs $\sin(\omega x), \cos(\omega x)$ and $x\sin(\omega x), x\cos(\omega x)$.

$$a_1 = -2, \quad b_0 = \frac{2\tan(\theta/2) - \theta}{\theta^3}, \quad b_1 = \frac{2[\theta - 2\tan(\theta/2)\cos(\theta)]}{\theta^3},$$

$$lte_{S_2} = h^6 \frac{\theta\sin(\theta) - 4(\cos(\theta)-1)^2}{\theta^3\sin(\theta)} \times [\omega^4 y''(x_n) + 2\omega^2 y^{(4)}(x_n) + y^{(6)}(x_n)]. \tag{7}$$

- S_3, integrating exactly the six functions $\sin(\omega x), \cos(\omega x), x\sin(\omega x), x\cos(\omega x), x^2\sin(\omega x), x^2\cos(\omega x)$.

$$a_1 = -\frac{2[2\theta + \cos(\theta)[3\sin(\theta) - \theta\cos(\theta)]]}{D},$$

$$b_0 = \frac{\sin(\theta) - \theta\cos(\theta)}{\theta^2 D},$$

$$b_1 = \frac{2[2\theta - \cos(\theta)[\sin(\theta) + \theta\cos(\theta)]]}{\theta^2 D}, \quad \text{with } D = 3\sin(\theta) + \theta\cos(\theta),$$

$$lte_{S_3} = -h^6 \frac{N}{F}[\omega^6 y(x_n) + 3\omega^4 y^{(2)}(x_n) + 3\omega^2 y^{(4)}(x_n) + y^{(6)}(x_n)],$$

$$\text{with } N = 6\frac{\sin(\theta)}{\theta} + 2\cos(\theta) - 6\cos(\theta)\frac{\sin(\theta)}{\theta} + 2\cos^2(\theta) - 4 \text{ and } F = \theta^6 D. \tag{8}$$

The relative merits of each of the four versions can be evaluated by comparing the expressions of the *lte*. It is seen that all *lte*s have one and the same h^6 dependence such that the order of each version is four. Also the factors in the middle are close to $-\frac{1}{240}$ when θ is around zero. The difference in accuracy can be expected to be in the third factor.

Results obtained for the eigenvalues by the classical Numerov method S_0 have properties described by (3). Those obtained by the so-called modified Numerov methods are identical with the ones derived by S_1. The error on these eigenvalues ${}^{(1)}\Sigma_k^{(n)}$ are given by (5). For the schemes S_2 and S_3 no analysis has been made up to now for eigenvalues related to bounded states. For resonance eigenenergies it has been shown in [17] that the way in which the errors increase with the energy differs from one version to another: S_3 delivers much more accurate results than S_2, which produces itself better results than S_1, which itself is superior over S_0.

3. Notations and preliminaries

By using the parameter values of the schemes S_2 and S_3 and a uniform mesh length $h := \pi/(n+1)$, the eigenvalues $\lambda_1, \ldots, \lambda_n$ of (1) are approximated by the eigenvalues ${}^{(i)}\Sigma_1^{(n)} < \cdots < {}^{(i)}\Sigma_k^{(n)}$, $i = 2, 3$ of the generalized algebraic eigenvalue problem

$$-{}^{(i)}A\,{}^{(i)}\mathbf{v} + {}^{(i)}B\,Q\,{}^{(i)}\mathbf{v} = {}^{(i)}\Sigma\,{}^{(i)}B\,{}^{(i)}\mathbf{v}, \tag{9}$$

where ${}^{(i)}A := ({}^{(i)}a_{ij})$ and ${}^{(i)}B := ({}^{(i)}b_{ij})$ are symmetric tridiagonal with

$$ {}^{(2)}a_{ii} := -\frac{2}{h^2} \ \ (i=1,\ldots,n), \quad {}^{(2)}a_{ii\pm 1} := \frac{1}{h^2} \ \ (i=1,\ldots,n-1), \tag{10} $$

$$ {}^{(3)}a_{ii} = -\frac{2[2\theta + \cos(\theta)[3\sin(\theta) - \theta\cos(\theta)]]}{3\sin(\theta) + \theta\cos(\theta)} \ \ (i=1,\ldots,n), $$

$$ {}^{(3)}a_{ii\pm 1} := \frac{1}{h^2} \quad (i=1,\ldots,n-1), \tag{11} $$

$$ {}^{(2)}b_{ii} := \frac{2[\theta - 2\tan(\theta/2)\cos(\theta)]}{\theta^3}, \quad {}^{(2)}b_{ii\pm 1} := \frac{2\tan(\theta/2) - \theta}{\theta^3}, \tag{12} $$

$$ {}^{(3)}b_{ii} := \frac{2[2\theta - \cos(\theta)[\sin(\theta) + \theta\cos(\theta)]]}{\theta^2 D}, $$

$$ {}^{(3)}a_{ii\pm 1} := \frac{\sin(\theta) - \theta\cos(\theta)}{\theta^2 D}, \tag{13} $$

and where

$$ Q := \mathrm{diag}(q(x_1),\ldots,q(x_n)) \quad \text{with } x_j := jh \ \ (j=1,\ldots,n). $$

When $q \equiv 0$ the corresponding algebraic eigenvalues (i.e. the eigenvalues of $(-{}^{(i)}B^{-1\,(i)}A),\ i=2,3$) are for both schemes, respectively, given by

$$ {}^{(2)}\mu_s^{(n)} = \frac{\theta^3[1-\cos(sh)]}{h^2[\theta(1-\cos(sh)) + 2\tan(\theta/2)(\cos(sh) - \cos(\theta))]}, \tag{14} $$

$$ {}^{(3)}\mu_s^{(n)} = \frac{2\theta^3 + 3\sin(\theta)\theta^2(\cos(\theta) - \cos(sh)) - \theta^3\cos(\theta)(\cos(\theta) + \cos(sh))}{h^2[2\theta + \sin(\theta)(\cos(sh) - \cos(\theta)) - \theta\cos(\theta)(\cos(sh) + \cos(\theta))]}, $$
$$ s = 1,2,\ldots,n. \tag{15} $$

The corresponding eigenvectors are in both cases

$$ w_s^{(n)} = (\sin(sx_1),\ldots,\sin(sx_n))^{\mathrm{T}}, \ \ (s=1,2,\ldots,n). \tag{16} $$

It is clear that by choosing $\omega = s$, $(s=1,2,\ldots,n)$, ${}^{(i)}\mu_s^{(n)}$, $(i=2,3)$ coincides with the exact eigenvalues $\lambda_s = s^2$ of (1) for $q=0$.

It is well known [11] that for general q the exact eigenvalues of (1) are given, under the assumption that $\int_0^\pi q(x)\,\mathrm{d}t = 0$ by

$$ \lambda_l = l^2 + \mathcal{O}(l^{-2}) \quad (l=1,2,3,\ldots). $$

Paine et al. [20] also proved that for $q \neq 0$ the general eigenfunctions of (1) corresponding to λ_l are given by

$$ y_l(x) = C_l \sin(lx) + \frac{1}{l}\int_0^x (l^2 - \lambda_l + q(x)) \sin l(x-t)\, y_l(x)\,\mathrm{d}t, \quad l=1,2,3\ldots\ , \tag{17} $$

where since y_l is arbitrary up to a scalar multiple, we can set $C_l = 1$, $(l=1,2,3\ldots)$. For further use we denote (17) as

$$ y_l(x) = \sin lx + e_l(x), \quad l=1,2,\ldots\ . \tag{18} $$

Since

$$ e_l^{(j)} = \mathcal{O}(l^{j-1}), \quad j=0,1,2,\ldots \tag{19} $$

the sine function is a first order approximation for $y(x)$.

Since S_2 and S_3 both integrate $\sin(\omega x)$, ω arbitrary and real, exactly, one can expect that (9) yields satisfactory approximations for the l-eigenvalues λ_l when we choose

$$\omega = l, \quad l = 1, 2, 3, \ldots .$$

As it was the case for S_1 one can formulate the following theorem:

Theorem. *If* $q \in \mathbb{C}^4[0, \pi]$ *there exists for the algorithms* S_i *a constant* $c^{(i)}$ *and a number* $\alpha \in (0, 1)$, *both depending only on* q *such that for all* $m \in \mathbb{N}$, $k = 1, 2, \ldots, m$ *and* $\omega = k$

$$|{}^{(i)}\Sigma_k^{(n)} - \lambda_k| \leqslant c^{(i)} k^3 h^4, \quad 1 \leqslant k \leqslant \alpha n, \quad i = 2, 3. \tag{20}$$

4. Proof of the theorem

We follow an approach inspired by the proofs in [7] and [22]. Many parts of the proof are identical for both algorithms. Where necessary we shall diversify and give separate treatments for S_2 and S_3, respectively.

Since for $i = 2$ and 3 ${}^{(i)}A$ and ${}^{(i)}B$ are symmetric commuting invertible matrices, we have

$${}^{(i)}A\,{}^{(i)}B^{-1} = {}^{(i)}B^{-1}\,{}^{(i)}A = ({}^{(i)}B^{-1}\,{}^{(i)}A)^{\mathrm{T}}.$$

Hence by (9)

$$-{}^{(i)}\mathbf{v}^{\mathrm{T}}\,{}^{(i)}B^{-1}\,{}^{(i)}A + {}^{(i)}\mathbf{v}^{\mathrm{T}} Q = {}^{(i)}\Sigma\,{}^{(i)}\mathbf{v}^{\mathrm{T}}.$$

Then by (1)

$$\begin{aligned} {}^{(i)}\Sigma\,{}^{(i)}\mathbf{v}^{\mathrm{T}}\mathbf{y} + {}^{(i)}\mathbf{v}^{\mathrm{T}}\,{}^{(i)}B^{-1}\,{}^{(i)}A\mathbf{y} &= {}^{(i)}\mathbf{v}^{\mathrm{T}} Q\mathbf{y} \\ &= \lambda\,{}^{(i)}\mathbf{v}^{\mathrm{T}}\mathbf{y} + {}^{(i)}\mathbf{v}^{\mathrm{T}}\mathbf{y}'', \end{aligned}$$

that is

$$\left({}^{(i)}\Sigma - \lambda\right){}^{(i)}\mathbf{v}^{\mathrm{T}}\mathbf{y} = {}^{(i)}\mathbf{v}^{\mathrm{T}}(\mathbf{y}'' - {}^{(i)}B^{-1}\,{}^{(i)}A\mathbf{y}). \tag{21}$$

Due to (18) with $l = k$, $(l = 1, 2, \ldots)$ one has

$$y_k''(x) = -k^2 \sin(kx) + e_k''(x) = -k^2 w_k(x) + e_k''(x) \quad (k = 1, 2, \ldots), \tag{22}$$

and from (18), (15) and (16), for $s = k$ and $\omega = k$ one finds

$$-{}^{(i)}B^{-1}\,{}^{(i)}A\mathbf{w}_k = k^2\mathbf{w}_k \quad (k = 1, 2, \ldots). \tag{23}$$

It follows from (18) and (21)–(23) that

$$({}^{(i)}\Sigma_k - \lambda_k)\,{}^{(i)}\mathbf{v}_k^{\mathrm{T}}\mathbf{y}_k = {}^{(i)}\mathbf{v}_k^{\mathrm{T}}(-k^2\mathbf{w}_k + \mathbf{e}_k'' - {}^{(i)}B^{-1}\,{}^{(i)}A\mathbf{e}_k + k^2\mathbf{w}_k)$$

or

$$\begin{aligned} ({}^{(i)}\Sigma_k - \lambda_k)\,{}^{(i)}\mathbf{v}_k^{\mathrm{T}}\mathbf{y}_k &= {}^{(i)}\mathbf{v}_k^{\mathrm{T}}(\mathbf{e}_k'' - {}^{(i)}B^{-1}\,{}^{(i)}A\mathbf{e}_k) \\ &= {}^{(i)}\boldsymbol{\epsilon}_k^{\mathrm{T}}(\mathbf{e}_k'' - {}^{(i)}B^{-1}\,{}^{(i)}A\mathbf{e}_k) \\ &\quad + \mathbf{w}_k^{\mathrm{T}}(\mathbf{e}_k'' - {}^{(i)}B^{-1}\,{}^{(i)}A\mathbf{e}_k) \quad (k = 1, 2, \ldots), \end{aligned} \tag{24}$$

where

$${}^{(i)}\boldsymbol{\epsilon}_k = {}^{(i)}\mathbf{v}_k - \mathbf{w}_k. \tag{25}$$

The following lemmas enable us to estimate the two terms in (24). We assume $\mathbf{y}_k$ normalized as in [20], with analogous normalization of ${}^{(i)}\mathbf{v}_k$. From here on, for reason of simplicity of notation we also omit the subscript k in all vectors.

Lemma 1.

$$||^{(i)}\boldsymbol{\epsilon}||_\infty \leqslant 2h\pi||q||_\infty||^{(i)}\mathbf{v}||_\infty/\sin(kh), \quad i=2,3.$$

Proof. Subtracting for $i=2$ or 3 $k^{2(i)}B^{(i)}\mathbf{v}+{}^{(i)}BQ^{(i)}\mathbf{v}$ from both sides of (9) yields

$$-{}^{(i)}A^{(i)}\mathbf{v}-k^{2(i)}B^{(i)}\mathbf{v}=({}^{(i)}\Sigma_k-k^2)^{(i)}B^{(i)}\mathbf{v}-{}^{(i)}BQ^{(i)}\mathbf{v}$$

or

- for S_2

$$\begin{aligned}&-\frac{1}{h^2}({}^{(2)}v_{j-1}-2^{(2)}v_j+{}^{(2)}v_{j+1})\\&-k^2\left[\left(\frac{2\tan(\theta/2)}{\theta^3}-\frac{1}{\theta^2}\right)({}^{(2)}v_{j+1}+{}^{(2)}v_{j-1})+\left(\frac{2}{\theta^2}-\frac{4\tan(\theta/2)\cos(\theta)}{\theta^3}\right){}^{(2)}v_j\right]\\&\quad=(({}^{(2)}\Sigma_k-k^2)^{(2)}B^{(2)}v-{}^{(2)}BQ^{(2)}v)_j,\end{aligned}$$

or

$$({}^{(2)}v_{j-1}-2\cos(\theta)^{(2)}v_j+{}^{(2)}v_{j+1})=\frac{kh^3}{2\tan(\theta/2)}((k^2-{}^{(2)}\Sigma_k)^{(2)}B^{(2)}v+{}^{(2)}BQ^{(2)}v)_j.$$

- for S_3

$$\begin{aligned}&-\frac{1}{h^2}\left({}^{(3)}v_{j-1}-\frac{2[2\theta+\cos(\theta)(3\sin(\theta)-\theta\cos(\theta))]}{3\sin(\theta)+\theta\cos(\theta)}{}^{(3)}v_j+{}^{(3)}v_{j+1}\right)\\&-k^2\left[\frac{\sin(\theta)-\theta\cos(\theta)}{\theta^2(3\sin(\theta)+\theta\cos(\theta))}({}^{(3)}v_{j+1}+{}^{(3)}v_{j-1})+\frac{2(2\theta-\cos(\theta)(\sin(\theta)+\theta\cos(\theta)))}{\theta^2(3\sin(\theta)+\theta\cos(\theta))}{}^{(3)}v_j\right]\\&\quad=(({}^{(3)}\Sigma_k-k^2)^{(3)}B^{(3)}v-{}^{(3)}BQ^{(3)}v)_j,\end{aligned}$$

or

$$\begin{aligned}&({}^{(3)}v_{j-1}-2\cos(\theta)^{(3)}v_j+{}^{(3)}v_{j+1})\\&\quad=\frac{h^2(3\sin(\theta)+\theta\cos(\theta))}{4\sin(\theta)}((k^2-{}^{(3)}\Sigma_k)^{(3)}B^{(3)}v+{}^{(3)}BQ^{(3)}v)_j.\end{aligned}$$

From Lemma 2.3 of [20] it then follows that

- for S_2

$$\begin{aligned}{}^{(2)}\varepsilon_j=&\frac{kh^3}{2\tan(\theta/2)\sin(\theta)}\sum_{i=1}^{j-1}\sin[k(x_j-x_i)]\\&\times\left[\left(\frac{2\tan(\theta/2)}{\theta^3}-\frac{1}{\theta^2}\right)((k^2-{}^{(2)}\Sigma_k+q_{i-1})^{(2)}v_{i-1}+(k^2-{}^{(2)}\Sigma_k+q_{i+1})^{(2)}v_{i+1})\right.\\&\left.+\left(\frac{2}{\theta^2}-\frac{4\tan(\theta/2)\cos(\theta)}{\theta^3}\right)(k^2-{}^{(2)}\Sigma_k+q_i)^{(2)}v_i\right],\end{aligned}$$

- for S_3

$$
\begin{aligned}
{}^{(3)}\varepsilon_j = {} & \frac{h^2(3\sin(\theta)+\theta\cos(\theta))}{4\sin^2(\theta)}\sum_{i=1}^{j-1}\sin[k(x_j-x_i)] \\
& \times\left[\frac{\sin(\theta)-\theta\cos(\theta)}{\theta^2(3\sin(\theta)+\cos(\theta))}((k^2-{}^{(3)}\Sigma_k+q_{i-1})^{(3)}v_{i-1}\right. \\
& +(k^2-{}^{(3)}\Sigma_k+q_{i+1})^{(3)}v_{i+1}) \\
& \left.+\frac{2[2\theta-\cos(\theta)(\sin(\theta)+\theta\cos(\theta))]}{\theta^2(3\sin(\theta)+\cos(\theta))}(k^2-{}^{(3)}\Sigma_k+q_i)^{(3)}v_i{}^{(3)}v_i\right].
\end{aligned}
$$

It is quite easy to verify that

$$
\begin{aligned}
&\frac{kh^3}{2\tan(\theta/2)\sin(\theta)}\left(\frac{2\tan(\theta/2)}{\theta^3}-\frac{1}{\theta^2}\right)=\frac{h^2}{12\sin(\theta)}+\mathcal{O}(h^4),\\
&\frac{\sin(\theta)-\theta\cos(\theta)}{4k^2\sin^2(\theta)}=\frac{h^2}{12\sin(\theta)}+\mathcal{O}(h^4),\\
&\frac{kh^3}{2\tan(\theta/2)\sin(\theta)}\left(\frac{2}{\theta^2}-\frac{4\tan(\theta/2)\cos(\theta)}{\theta^3}\right)=\frac{5h^2}{6\sin(\theta)}+\mathcal{O}(h^4),\\
&\frac{2[2\theta-\cos(\theta)(\sin(\theta)+\theta\cos(\theta))]}{4k^2\sin^2(\theta)}=\frac{5h^2}{6\sin(\theta)}+\mathcal{O}(h^4),
\end{aligned}
$$

so that for both algorithms

$$
\begin{aligned}
{}^{(i)}\varepsilon_j = {} & \frac{h^2}{12\sin(\theta)}\sum_{m=1}^{j-1}\sin[k(x_j-x_m)] \\
& \times\left[(k^2-{}^{(i)}\Sigma_k+q_{m-1})^{(i)}v_{m-1}+10(k^2-{}^{(i)}\Sigma_k+q_m)^{(i)}v_m\right. \\
& \left.+(k^2-{}^{(i)}\Sigma_k+q_{m+1})^{(i)}v_{m+1}\right]+\mathcal{O}(h^4)\quad\text{for } i=2,3. \qquad (26)
\end{aligned}
$$

Since ${}^{(i)}B^{-1(i)}A$, for $i=2, 3$, and Q are real symmetric it follows from (9) and $-{}^{(i)}A\mathbf{w}_k^{(n)}={}^{(i)}\mu_k^{(n)}\mathbf{w}_k^{(n)}$ and standard perturbation theory [23, p. 102] that

$$
|k^2-{}^{(i)}\Sigma_k|\leqslant||Q||_\infty=||\mathbf{q}||_\infty.
$$

Hence by (26) and the triangle inequality

$$
\begin{aligned}
|{}^{(i)}\varepsilon_j| &\leqslant\left|\frac{h^2(j-1)}{\sin(kh)}\right|\max_i(|k^2-{}^{(i)}\Sigma_k+q_i||{}^{(i)}v_i|)\\
&\leqslant\left[\frac{2(j-1)h^2}{\sin(kh)}\right]||\mathbf{q}||_\infty||{}^{(\mathbf{i})}\mathbf{v}||_\infty\\
&\leqslant\left[\frac{2\pi h}{\sin(kh)}\right]||q||_\infty||{}^{(i)}\mathbf{v}||_\infty,
\end{aligned}
$$

since $h(j-1)\leqslant\pi$. □

Lemma 2. *Let*

$$f := (k^2 - \lambda_k + q)y,$$

$$\alpha(x,h) := \int_x^{x+h} f(t)\sin[k(x-h-t)]\,\mathrm{d}t \tag{27}$$

and

$$E_j := \alpha(x_j, h) + \alpha(x_j, -h), \tag{28}$$

then

- *for* S_2:

$$^{(2)}A\mathbf{e} - {}^{(2)}B\mathbf{e}'' = \frac{2\tan(\theta/2)}{k^2h^3}\mathbf{E} - {}^{(2)}B\mathbf{f}, \tag{29}$$

- *for* S_3:

$$^{(3)}A\mathbf{e} - {}^{(3)}B\mathbf{e}'' = \frac{4\sin(\theta)}{kh^2(3\sin(\theta)+\theta\cos(\theta))}\mathbf{E} - {}^{(3)}B\mathbf{f}. \tag{30}$$

Proof. Due to the definition of $e(x)$ (see (17)–(18))

$$e'' = f - k^2 e$$

and hence

$$^{(i)}B\mathbf{e}'' = {}^{(i)}B\mathbf{f} - k^{2\,(i)}B\mathbf{e} \quad (i = 2, 3). \tag{31}$$

- For S_2: by (10), (17), (18) and (28)

$$\begin{aligned} kh^2({}^{(2)}A\mathbf{e})_j &= k(e_{j+1} - 2e_j + e_{j-1}) \\ &= \int_0^{x_j} f(t)[\sin k(x_{j+1}-t) - 2\sin k(x_j - t) + \sin k(x_{j-1}-t)]\,\mathrm{d}t + E_j \\ &= -k^2h^2\int_0^{x_j} f(t)\left(-\frac{1}{\theta^2}\right)[\sin k(x_{j+1}-t) - 2\sin k(x_j-t) + \sin k(x_{j-1}-t)]\,\mathrm{d}t \\ &\quad - k^2h^2\int_0^{x_j} f(t)\left[\frac{2\tan(\theta/2)}{\theta^3}(\sin k(x_{j+1}-t) + \sin k(x_{j-1}-t))\right. \\ &\quad \left. - \frac{4\tan(\theta/2)\cos(\theta)}{\theta^3}\sin k(x_j - t)\right]\mathrm{d}t + E_j \\ &= -k^2h^2\int_0^{x_j} f(t) \\ &\quad [{}^{(2)}b_{jj+1}\sin k(x_{j+1}-t) + {}^{(2)}b_{jj}\sin k(x_j-t) + {}^{(2)}b_{jj-1}\sin k(x_{j-1}-t)]\,\mathrm{d}t + E_j \\ &= -h^2k^3[{}^{(2)}b_{jj+1}e_{j+1}{}^{(2)}b_{jj}e_j + {}^{(2)}b_{jj-1}e_{j-1}] + E_j\left(1 + h^2k^2\left(\frac{2\tan(\theta/2)}{\theta^3} - \frac{1}{\theta^2}\right)\right). \end{aligned}$$

Hence

$$A\mathbf{e} = -k^{2\,(2)}B\mathbf{e} + \frac{2k\tan(\theta/2)}{k^2h^3}\mathbf{E}. \tag{32}$$

Substracting (31) from (32) gives (29).

- For S_3: by (11), (17), (18) and (28)

$$
\begin{aligned}
kh^2({}^{(3)}Ae)_j &= k\left(e_{j+1} - \frac{2(2\theta+\cos(\theta)(3\sin(\theta)-\theta\cos(\theta)))}{3\sin(\theta)+\theta\cos(\theta)}e_j + e_{j-1}\right)\\
&= \int_0^{x_j} f(t)\left[\sin k(x_{j+1}-t) - \frac{2(2\theta+\cos(\theta)(3\sin(\theta)-\theta\cos(\theta)))}{3\sin(\theta)+\theta\cos(\theta)}\sin k(x_j-t)\right.\\
&\quad\left. +\ \sin k(x_{j-1}-t)\right]\mathrm{d}t + E_j\\
&= -\int_0^{x_j} f(t)\frac{4\theta\sin^2(\theta)}{3\sin(\theta)+\theta\cos(\theta)}\sin k(x_j-t)\,\mathrm{d}t + E_j\\
&= -k^2h^2\int_0^{x_j} f(t)[{}^{(3)}b_{jj}\sin k(x_j-t) + {}^{(3)}b_{jj+1}\,2\cos(\theta)\sin k(x_j-t)]\,\mathrm{d}t + E_j\\
&= -k^2h^2\int_0^{x_j} f(t)\\
&\quad\times\left[{}^{(3)}b_{jj+1}\sin k(x_{j+1}-t) + {}^{(3)}b_{jj}\sin k(x_j-t) + {}^{(3)}b_{jj-1}\sin k(x_{j-1}-t)\right]\mathrm{d}t + E_j\\
&= -h^2k^3[{}^{(3)}b_{jj+1}e_{j+1} + {}^{(3)}b_{jj}e_j + {}^{(3)}b_{jj-1}e_{j-1}]\\
&\quad + E_j\left(1+h^2k^2\left(\frac{4\sin(\theta)}{\theta^2(3\sin(\theta)+\theta\cos(\theta)} - \frac{1}{\theta^2})\right)\right).
\end{aligned}
$$

Hence

$$
A\mathbf{e} = -k^{2\,(2)}B\mathbf{e} + \frac{4\tan(\theta)}{kh^2(3\sin(\theta)+\theta\cos(\theta))}\mathbf{E}. \tag{33}
$$

Subtracting (31) from (33) gives (30). □

Lemma 3. *For all $q \in \mathbb{C}^4[0,\pi]$ there exists a constant $d^{(i)}$ such that*

$$
|{}^{(i)}\varepsilon^{\mathrm{T}}[{}^{(i)}B^{-1\,(i)}A\mathbf{e} - \mathbf{e}'']| \leqslant d^{(i)}h^4k^4/\sin(kh), \quad k = 1,2,\ldots,n, \quad i = 2,3.
$$

Proof. By (28) and (27)

$$
E_j = \int_{x_j}^{x_{j+1}} f(t)\sin k(x_{j+1}-t)\,\mathrm{d}t + \int_{x_j}^{x_{j+1}} f(t)\sin k(x_{j-1}-t)\,\mathrm{d}t.
$$

Expanding f about x_j by Taylor's theorem in both integrals and integrating by parts shows that

$$
\begin{aligned}
\mathbf{E} &= \frac{2}{k}(1-\cos(\theta))\mathbf{f} + \left[\frac{h^2}{k} - \frac{2}{k^3}(1-\cos(\theta))\right]\mathbf{f}''\\
&\quad + \left[\frac{h^4}{12k} - \frac{h^2}{k^3} + \frac{2}{k^5}(1-\cos(\theta))\right]\mathbf{f}^{(iv)} + \mathbf{O}(h^6).
\end{aligned} \tag{34}
$$

- For S_2: also

$$
({}^{(2)}B\mathbf{f})_j = \frac{4\tan(\theta/2)}{\theta^3}(1-\cos(\theta))f_j + (h^2 f_j'' + \frac{h^4}{12}f_j^{(iv)})\left(\frac{2\tan(\theta/2)}{\theta^3} - \frac{1}{\theta^2}\right) + \mathcal{O}(h^6). \tag{35}
$$

Combining (29), (34) and (35) yields

$$\begin{aligned}
{}^{(2)}A\mathbf{e} - {}^{(2)}B\mathbf{e}'' &= \frac{2\tan(\theta/2)}{k^2h^3}\mathbf{E} - {}^{(2)}B\mathbf{f} \\
&= \mathbf{f}''\left[\frac{1}{k^2} - \frac{4\tan(\theta/2)}{k^5h^3}(1-\cos(\theta))\right] \\
&\quad + \mathbf{f}^{(iv)}\left[\frac{h^4}{12k} - \frac{h^2}{k^3} + \frac{2}{k^5}(1-\cos(\theta)) - \frac{h^4}{12}\left(\frac{2\tan(\theta/2)}{\theta^3} - \frac{1}{\theta^2}\right) + \mathcal{O}(h^6)\right] \\
&= \mathbf{f}''(\mathcal{O}(k^2h^4)) + \mathbf{f}^{(iv)}(\mathcal{O}(h^4)) = \mathcal{O}(k^4h^4) \qquad (36)
\end{aligned}$$

since $\mathcal{O}(||\mathbf{f}^p||_\infty) = \mathcal{O}(k^p)$.

- For S_3:

$$\begin{aligned}
({}^{(3)}B\mathbf{f})_j &= \frac{4\theta + \sin(\theta)(2-2\cos(\theta)) - \theta\cos(\theta)(2+2\cos(\theta))}{\theta^2(3\sin(\theta)+\theta\cos(\theta))} f_j \\
&\quad + \left(h^2 f_j'' + \frac{h^4}{12} f^{(iv)}\right)\left(\frac{4\sin(\theta)}{\theta^2(3\sin(\theta)+\theta\cos(\theta))} - \frac{1}{\theta^2} + \mathcal{O}(h^6)\right). \qquad (37)
\end{aligned}$$

Combining (30), (34) and (37) yields

$$\begin{aligned}
{}^{(3)}A\mathbf{e} - {}^{(3)}B\mathbf{e}'' &= \frac{4\sin(\theta)}{kh^2(3\sin(\theta)+\theta\cos(\theta))}\mathbf{E} - {}^{(2)}B\mathbf{f} \\
&= \mathbf{f}\frac{\sin(\theta)(1-\cos(\theta)) - 4\theta + \sin(\theta)(2-2\cos(\theta)) - \theta\cos(\theta)(2+2\cos(\theta))}{\theta^2(3\sin(\theta)+\theta\cos(\theta))} \\
&\quad + \mathbf{f}''\left(\frac{1}{k^2} - \frac{8\sin(\theta)(1-\cos(\theta))}{k^4h^2(3\sin(\theta)+\theta\cos(\theta))}\right) \\
&\quad + \mathbf{f}^{(iv)}\left(\frac{h^2}{12k^2} + \frac{4\sin(\theta)}{kh^2(3\sin(\theta)+\theta\cos(\theta))}\left(-\frac{h^2}{k^3} + \frac{2}{k^5}(1-\cos(\theta))\right)\right)
\end{aligned}$$

which by the help of series expansion reduces to

$$\begin{aligned}
{}^{(3)}A\mathbf{e} - {}^{(3)}B\mathbf{e}'' &= \mathbf{f}\left(-\frac{k^4h^4}{240} - \frac{k^6h^6}{2016} + \mathcal{O}(h^8)\right) \\
&\quad + \mathbf{f}''\left(-\frac{k^2h^4}{120} - \frac{71\,k^4h^6}{60480} + \mathcal{O}(h^8)\right) \\
&\quad + \mathbf{f}^{(iv)}\left(-\frac{h^4}{240} - \frac{13\,k^3h^6}{15120} + \mathcal{O}(h^8)\right) \\
&= \mathcal{O}(k^4h^4). \qquad (38)
\end{aligned}$$

Since also

$$|{}^{(i)}\boldsymbol{\epsilon}^{\mathrm{T}}({}^{(i)}B^{(-1)}{}^{(i)}A\mathbf{e} - \mathbf{e}'')| \leqslant n||{}^{(i)}\boldsymbol{\epsilon}||_\infty||{}^{(i)}B^{(-1)}||_\infty||{}^{(i)}A\mathbf{e} - {}^{(i)}B\mathbf{e}''||_\infty, \quad i = 2, 3$$

and

$$n = \mathcal{O}\left(\frac{1}{h}\right), \quad ||^{(i)}B^{(-1)}||_\infty = \mathcal{O}(1), \quad i = 2, 3,$$

the result follows from Eqs. (36) and (38) and Lemmas 1 and 2. □

It is easy to verify that due to (14)–(16), $\omega = s = k$, $(k = 1, \ldots, n)$, $\theta = kh$:

$$\mathbf{w}^{\mathrm{T}}(\mathbf{e}'' - {}^{(i)}B^{-1(i)}A\mathbf{e}) = \mathbf{w}^{\mathrm{T}}(\mathbf{e}'' + k^2\mathbf{e}) = \mathbf{w}^{\mathrm{T}}\mathbf{f}.$$

Lemma 4. *Under the assumption that* $q(x) \in \mathbb{C}^4[0, \pi]$

$$\mathbf{w}^{\mathrm{T}}\mathbf{f}' < c'k^4h^4/\sin(\theta).$$

The proof is omitted, since it is essentially the same as the proof of Lemma 6 of [7]. □

By Lemma 1 and (17), $||\mathbf{v} - \mathbf{w}||_\infty$ and $||\mathbf{y} - \mathbf{w}||_\infty$ are both $\mathcal{O}(k^{-1})$ for large k. Hence, since $(\mathbf{w}^{\mathrm{T}}\mathbf{w})^{-1} = \mathcal{O}(h)$, there exist positive constants k_0 and c'' such that

$$\mathbf{v}^{\mathrm{T}}\mathbf{y} \geqslant c''/h, \quad \forall k \geqslant k_0. \tag{39}$$

Combining (24), (39) with the results of Lemmas 3 and 4 proves the theorem for $k \geqslant k_0$.

For $k \leqslant k_0$ we can lean on (7) and (8), respectively, to state that the ith component of

$$(-{}^{(i)}A + {}^{(i)}BQ - \lambda_k{}^{(i)}B)\mathbf{y}, \quad i = 2, 3$$

is given by

- for S_2:

$$h^6\,\frac{\theta\sin(\theta) - 4(\cos(\theta) - 1)^2}{\theta^3\sin(\theta)}[\omega^4 y''(\eta_p) + 2\omega^2 y^{(4)}(\eta_p) + y^{(6)}(\eta_p)],$$

- for S_3:

$$-h^6\,\frac{N}{F}[\omega^6 y(\eta_p) + 3\omega^4 y^{(2)}(\eta_p) + 3\omega^2 y^{(4)}(\eta_p) + y^{(6)}(\eta_p)],$$

with $N = 6\,\dfrac{\sin(\theta)}{\theta} + 2\cos(\theta) - 6\cos(\theta)\,\dfrac{\sin(\theta)}{\theta} + 2\cos^2(\theta) - 4.$

and $F = \theta^6 D$ and $D = 3\sin(\theta) + \theta\cos(\theta)$,

where $|\eta_p - x_p| < h$, $(p = 1, \ldots, n)$. One can easily prove that

$$(-{}^{(i)}A + {}^{(i)}BQ - \lambda_k{}^{(i)}B)\mathbf{y} = \mathcal{O}(k^4h^4||\mathbf{y}||_\infty), \quad i = 2, 3$$

since

$$h^6\,\frac{\theta\sin(\theta) - 4(\cos(\theta) - 1)^2}{\theta^3\sin(\theta)} = \mathcal{O}(h^4)$$

and also

$$-h^6\,\frac{N}{F} = \mathcal{O}(h^4)$$

and

$$\omega^4 y''(\eta_p) + 2\omega^2 y^{(4)}(\eta_p) + y^{(6)}(\eta_p) = \mathcal{O}(k^4\|\mathbf{y}\|_\infty),$$

and so is

$$\omega^6 y(\eta_p) + 3\omega^4 y^{(2)}(\eta_p) + 3\omega^2 y^{(4)}(\eta_p) + y^{(6)}(\eta_p) = \mathcal{O}(k^4\|\mathbf{y}\|_\infty).$$

By $\|{}^{(i)}B^{-1}\|_\infty = \mathcal{O}(1)$, $i = 2, 3$ and an analysis similar to that in [18, pp. 133–134], one can show that

$$|{}^{(i)}\Sigma_k^{(n)} - \lambda_k| = \mathcal{O}(h^4k^4), \quad i = 2, 3.$$

This result implies that there exist a constant c''' such that for $k < k_0$

$$|{}^{(i)}\Sigma_k^{(n)} - \lambda_k| \leqslant c''' h^4 k^4, \quad i = 2, 3. \qquad \square$$

5. Numerical experiments

In order to facilitate comparison with the results of [7] and [22], we choose the same functions q in (1) for our numerical examples, i.e. $q(x) = \exp(x)$ and $q(x) = (x + 0.1)^{-2}$. In Table 1 we compare for $q(x) = \exp(x)$ and for $n = 39$ the ${}^{(i)}\Sigma_k$, $i = 1, 2, 3$ as obtained with the algorithms S_1, S_2 and S_3 for $k = 1, 2, \ldots, n$. For the determination of the ${}^{(i)}\Sigma$ we have chosen $\omega = k$, $(k = 1, 2, \ldots, 39)$. It is clear that the errors are all of the same order as predicted by the theorem. The results obtained by S_3 are however a little more accurate than the ones obtained by S_2, which are again a little bit more accurate than those obtained by S_1. In Table 2 we present the analogous results for $q(x) = (x + 0.1)^{-2}$ again for $n = 39$. These results show that the errors for the three schemes behave identically. The presented errors as obtained by S_1, S_2 and S_3 are within a few percent equal. To confirm the theorem, Table 3 gives the values of $(\lambda_k - {}^{(i)}\Sigma_k^{(n)})/(k^3h^4)$, $i = 1, 2, 3$ with $q(x) = \exp(x)$ for $n = 19, 39, 79$.

Table 1
The errors ($\times 10^{+3}$) as obtained with the algorithms S_1, S_2, S_3 for $q(x) = e^x$

k	λ_k	$(\lambda_k - {}^{(1)}\Sigma_k) \times 10^3$	$(\lambda_k - {}^{(2)}\Sigma_k) \times 10^3$	$(\lambda_k - {}^{(3)}\Sigma_k) \times 10^3$
1	4.8966694	0.0019	0.0014	0.0009
2	10.045190	0.0215	0.0127	0.0061
3	16.019267	0.7515	0.0424	0.0130
4	23.266271	0.1717	0.1040	0.0287
5	32.263707	0.3051	0.1959	0.0599
6	43.220020	0.4714	0.3132	0.1069
7	56.181594	0.6694	0.4535	0.1663
8	71.152998	0.9028	0.6197	0.2391
9	88.132119	1.1720	0.8115	0.3235
10	107.11668	1.4860	1.0373	0.4265
11	128.10502	1.8343	1.2859	0.5354
12	151.09604	2.2331	1.5723	0.6638
13	176.08900	2.6939	1.9073	0.8204
14	203.08337	3.2022	2.2748	0.9873
15	232.07881	3.7797	2.6947	1.1819
16	263.07507	4.4366	3.1752	1.4095
17	296.07196	5.1758	3.7168	1.6671
18	331.06934	6.0046	4.3233	1.9545
19	368.06713	6.9597	5.0273	2.2994
20	407.06524	8.0476	5.8307	2.6973

Table 2
The errors ($\times 10^{+3}$) as obtained with the algorithms S_1, S_2, S_3 for $q(x) = 1/(x+0.1)^2$

k	λ_k	$(\lambda_k - {}^{(1)}\Sigma_k) \times 10^3$	$(\lambda_k - {}^{(2)}\Sigma_k) \times 10^3$	$(\lambda_k - {}^{(3)}\Sigma_k) \times 10^3$
1	1.5198658	0.0462	0.0461	0.0461
2	4.9433098	0.2914	0.2900	0.2889
3	10.284663	0.8945	0.8869	0.8809
4	17.559958	1.9831	1.9593	1.9403
5	26.782863	3.6530	3.5981	3.5531
6	37.964426	5.9748	5.8698	5.7807
7	51.113358	9.0003	8.8231	8.6675
8	66.236448	12.7734	12.5000	12.2518
9	83.338962	17.3348	16.9402	16.5698
10	102.42499	22.7309	22.1899	21.6651
11	123.49771	29.0072	28.2949	27.5808
12	146.55961	36.2192	35.3114	34.3712
13	171.61264	44.4243	43.2982	42.0929
14	198.65837	53.7188	52.3527	50.8451
15	227.69803	64.1866	62.5608	60.7012
16	258.73262	75.9416	74.0387	71.7862
17	291.76293	89.0972	86.9023	84.2107
18	326.78963	103.8191	101.3208	98.1421
19	363.81325	120.2784	117.4692	113.7536
20	402.83424	138.6931	135.5705	131.2667

Table 3
Scaled errors $(\lambda_k - {}^{(i)}\Sigma_k^{(n)})/(k^3 h^4)$ with $q(x) = \exp(x)$

k	$i=1$			$i=2$			$i=3$		
	$n=19$	$n=39$	$n=79$	$n=19$	$n=39$	$n=79$	$n=19$	$n=39$	$n=79$
1	0.0508	0.0512	0.0591	0.0352	0.0355	0.0434	0.0231	0.0235	0.0314
2	0.0708	0.0706	0.0757	0.0415	0.0415	0.0476	0.0198	0.0200	0.0252
3	0.0744	0.0731	0.0692	0.0421	0.0413	0.0375	0.0129	0.0127	0.0090
4	0.0723	0.0705	0.0704	0.0439	0.0427	0.0428	0.0118	0.0118	0.0121
5	0.0670	0.0641	0.0633	0.0432	0.0411	0.0405	0.0129	0.0125	0.0124
6	0.0614	0.0574	0.0570	0.0410	0.0381	0.0380	0.0138	0.0130	0.0134
7	0.0567	0.0512	0.0501	0.0388	0.0381	0.0381	0.0141	0.0127	0.0124
8	0.0533	0.0463	0.0452	0.0371	0.0318	0.0310	0.0143	0.0122	0.0122
9	0.0511	0.0512	0.0404	0.0359	0.0293	0.0278	0.0145	0.0116	0.0109
10		0.0393	0.0385		0.0272	0.0272		0.0112	0.0120
11		0.0362	0.0335		0.0254	0.0231		0.0106	0.0093
12		0.0340	0.0305		0.0239	0.0210		0.0101	0.0082
13		0.0322	0.0298		0.0228	0.0210		0.0098	0.0093
14		0.0306	0.0272		0.0217	0.0190		0.0095	0.0081
15		0.0294	0.0254		0.0209	0.0178		0.0092	0.0075
16		0.0284	0.0245		0.0203	0.0173		0.0090	0.0076
17		0.0277	0.0233		0.0198	0.0165		0.0089	0.0073
18		0.0270	0.0216		0.0195	0.0152		0.0088	0.0064
19		0.0266	0.0210		0.0192	0.0149		0.0088	0.0065

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