

Error Bounds and Estimates for Eigenvalues of Integral Equations

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Summary. Approximate solutions of the linear integral equation eigenvalue problem can be obtained by the replacement of the integral by a numerical quadrature formula and then collocation to obtain a linear algebraic eigenvalue problem. This method is often called the Nyström method and its convergence was discussed in [7]. In this paper computable error bounds and dominant error terms are derived for the approximation of simple eigenvalues of nonsymmetric kernels.

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1. Introduction

In an earlier paper [7] the author discussed the convergence of the Nyström method (quadrature method) for the approximate solution of the integral equation

$$\lambda x(s) = \int_a^b k(s, t) x(t) dt \tag{1}$$

where a and b are finite, $k(s, t)$ is known in $C[a, b] \times [a, b]$ and λ and $x(s)$ are unknowns. Equation (1) can be written

$$\lambda x = Kx \tag{2}$$

where $x \in X$, a linear space, and $K: X \rightarrow X$. Under certain conditions on $k(s, t)$ and with an appropriate norm on X , K is a compact operator in a Banach space X .

To obtain approximations to the solutions of (2), a related matrix equation can be set up using a quadrature rule to approximate the integral in (1), i.e.

$$\lambda^{(n)} \mathbf{u} = \mathbf{K}_n \mathbf{u} \tag{3}$$

where $\mathbf{u} \in E_n$, Euclidean n -space, and $\mathbf{K}_n: E_n \rightarrow E_n$.

In [5] and [7] a framework for an error analysis of the above approach was described. Prolongation and restriction operators, $p_n: E_n \rightarrow X$ and $r_n: X \rightarrow E_n$ were used to show that the solutions of (2) satisfy

$$\lambda r_n x = [\mathbf{K}_n + \mathbf{B}_n(\lambda)] r_n x \quad (4)$$

where

$$\mathbf{B}_n(\lambda) = r_n K p_n - \mathbf{K}_n + r_n K (\lambda - Q_n)^{-1} Q_n p_n \quad (5)$$

and

$$Q_n = (1 - p_n r_n) K \quad (6)$$

provided

$$|\lambda| > \|Q_n\|. \quad (7)$$

The importance of (7) is illustrated in Table 1.

Equation (4) is the key equation. If we can choose p_n and r_n so that $\|r_n K p_n - \mathbf{K}_n\| \rightarrow 0$ as $n \rightarrow \infty$, and $\|Q_n\| \rightarrow 0$ as $n \rightarrow \infty$ then for a fixed λ , $\|\mathbf{B}_n(\lambda)\| \rightarrow 0$ as $n \rightarrow \infty$ and the matrix in (4) can be regarded as a perturbation of the matrix in (3). A convergence analysis using this approach is given in [7]. It was proved that (provided K in (1) is compact) for a simple eigenvalue of (1) there is a simple eigenvalue, $v^{(n)}$ say, of (3) such that

$$|\lambda - v^{(n)}| \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

If \mathbf{u}_n is the corresponding eigenvector of $v^{(n)}$, suitably normalised, then

$$\|r_n x - \mathbf{u}_n\| \rightarrow 0 \quad \text{as } n \rightarrow \infty \quad (8)$$

and

$$\|p_n \mathbf{u}_n - x\| \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

We assume that, for all n

$$\|p_n\| \leq p, \quad \|r_n\| \leq r. \quad (9)$$

Such operators are said to be stable.

Most of the previous analysis for the Nyström method has relied on the kernel being symmetric or normal, notably Wielandt [11], Brakhage [2], and Keller [4]. Recently however results for non-hermitian kernels have been given by Atkinson [1], Bramble and Osborn [3], and Vainikko [10]. The results in this paper provide convergence rates and rigorous error bounds in a constructive manner which allows bounds and error terms to be readily estimated.

In Section 2 of this paper we obtain rigorous error bounds for the quantities $|\lambda - v^{(n)}|$ and $\|r_n x - \mathbf{u}_n\|$ which can be readily estimated. These bounds provide a convergence theorem for the numerical solution of (1) using the Nyström method. Dominant error terms are obtained in Section 3. In Sections 4–6 the theory is

illustrated by the analysis of the trapezoidal rule method applied to a certain integral equation. The bounds and error terms are explicitly calculated and their numerical performance discussed.

2. Error Bounds

Assume \mathbf{K}_n has distinct eigenvalues $v_i^{(n)}$ $i = 1, \dots, n$ with right and left eigenvectors \mathbf{u}_i and \mathbf{v}_i^H respectively. (As we note later, this assumption is easily weakened.) It is known that quantities s_i $i = 1, \dots, n$ exist which satisfy

$$\mathbf{v}_i^H \mathbf{u}_j = \begin{cases} s_i \neq 0 & i = j \\ 0 & i \neq j. \end{cases}$$

If the eigenvectors are normalised by

$$\|\mathbf{u}_i\|_\infty = 1 \quad \text{and} \quad \|\mathbf{v}_i\|_1 = 1 \tag{10}$$

then $|s_i| = |\mathbf{v}_i^H \mathbf{u}_i| \leq \|\mathbf{v}_i\|_1 \|\mathbf{u}_i\|_\infty = 1$. For a Hermitian matrix we can find eigenvectors such that $s_i = 1$ $i = 1, \dots, n$ and all the eigenvalues are ‘‘well conditioned’’. If an s_i is nearly zero then the eigenvalue is ‘‘badly conditioned’’. (See Wilkinson [12].) From now on $\|\cdot\|$ will mean $\|\cdot\|_\infty$ and any other norms will be explicitly labelled.

Consider any simple eigenvalue λ_i of (4) satisfying (7) with corresponding eigenvector $r_n \mathbf{x}_i = \mathbf{x}_i$. Since $\{\mathbf{u}_j\}_{j=1}^n$ span E_n , \mathbf{x}_i can be expressed in the form

$$\mathbf{x}_i = \mathbf{u}_i + \sum' \alpha_{ij} \mathbf{u}_j \tag{11}$$

where the prime indicates that the term $j = i$ is omitted from the sum and where \mathbf{u}_i is the eigenvector corresponding to $v_i^{(n)}$ in (3). [Equation (11) normalises \mathbf{x}_i and so, from (8), $\alpha_{ij} \rightarrow 0$ as $n \rightarrow \infty$.]

Substitute (11) in (4) and forming the inner product of the result with \mathbf{v}_k we obtain (dropping the superscript n from $v_j^{(n)}$)

$$(\lambda_i - v_i) s_i = b_{ii}(\lambda_i) + \sum' b_{ij}(\lambda_i) \alpha_{ij} \tag{12}$$

$$\alpha_{ik} (\lambda_i - v_k) s_k = b_{ki}(\lambda_i) + \sum' b_{kj}(\lambda_i) \alpha_{ij} \quad k = 1, \dots, i - 1, i + 1, \dots, n, \tag{13}$$

where $b_{pq}(\lambda_i) = \mathbf{v}_p^H \mathbf{B}_n(\lambda_i) \mathbf{u}_q$.

These equations are used to provide rigorous bounds for $|\lambda_i - v_i|$ and α_{ij} ($i \neq j$). Make the following change of variables.

$$\gamma_i = (\lambda_i - v_i) s_i \tag{14}$$

$$\gamma_k = (v_i - v_k) s_k \alpha_{ik} \quad k = 1, \dots, i - 1, i + 1, \dots, n \tag{15}$$

$$b_{pq}(\lambda_i) = b_{pq}(v_i + \gamma_i/s_i) = c_{pq}(\gamma_i) \quad p, q = 1, \dots, n. \tag{16}$$

Equations (12) and (13) become

$$\gamma_i = c_{ii}(\gamma_i) + \sum' \frac{c_{ij}(\gamma_i) \gamma_j}{(v_i - v_j) s_j}, \tag{17}$$

$$\gamma_k = c_{ki}(\gamma_i) + \sum_j' \frac{c_{kj}(\gamma_i) \gamma_j}{(v_i - v_j) s_j} - \frac{\gamma_i \gamma_k}{(v_i - v_k) s_i} \quad k = 1, \dots, i-1, i+1, \dots, n$$

which we write as

$$\gamma = \mathbf{c}_i(\gamma) + \mathbf{H}(\gamma) \gamma + \mathbf{M}(\gamma) \gamma \tag{18}$$

where $\gamma = [\gamma_1, \dots, \gamma_n]^T$, $\mathbf{c}_i(\gamma) = [c_{1i}(\gamma_i), \dots, c_{ni}(\gamma_i)]^T$

$$[\mathbf{H}(\gamma)]_{pq} = \begin{cases} \frac{c_{pq}(\gamma_i)}{(v_i - v_q) s_q} & q \neq i \\ 0 & \text{otherwise} \end{cases}$$

$$[\mathbf{M}(\gamma)]_{pq} = \begin{cases} \frac{-\gamma_q}{(v_i - v_q) s_q} & p = q \neq i \\ 0 & \text{otherwise.} \end{cases}$$

To obtain bounds for $\|\gamma\|$ we use the result of the following lemma.

Lemma. Let $\gamma, \mathbf{c}(\gamma) \in E_n$, Euclidean n space, and $\mathbf{H}(\gamma)$ and $\mathbf{M}(\gamma)$ be $n \times n$ matrices with elements depending on γ .

Assume D is the closed ball

$$D = \left\{ \gamma: \|\gamma\| \leq \frac{\|\mathbf{c}(\mathbf{0})\|}{1 - C_1 - H_0} w(g) \right\}$$

where

(i) $\mathbf{c}(\gamma)$, $\mathbf{H}(\gamma)$ and $\mathbf{M}(\gamma)$ satisfy Lipschitz conditions in D with Lipschitz constants C_1, H_1, M_1 respectively,

(ii) $\|\mathbf{H}(\mathbf{0})\| = H_0$ and $\mathbf{M}(\mathbf{0}) = \mathbf{0}$,

(iii) $1 - C_1 - H_0 > 0$,

(iv) $g = \frac{2(H_1 + M_1) \|\mathbf{c}(\mathbf{0})\|}{(1 - C_1 - H_0)^2} < \frac{1}{2}$ and $w(g) = \frac{1 - \sqrt{1 - 2g}}{g}$.

Then

$$\gamma = \mathbf{c}(\gamma) + \mathbf{H}(\gamma) \gamma + \mathbf{M}(\gamma) \gamma$$

has a unique solution in D .

Proof. Introduce F , a mapping on E_n , defined by

$$F(\gamma) = \mathbf{c}(\gamma) + \mathbf{H}(\gamma) \gamma + \mathbf{M}(\gamma) \gamma.$$

It is straightforward to show

(i) $F(D) \subset D$,

(ii) F is a contraction mapping on D

and a standard theorem [6, p. 120] gives the required result. Q.E.D.

To apply the result of this lemma we need to find $\|\mathbf{c}_i(\mathbf{0})\|_\infty, C_1, H_0, H_1$ and M_1 . Using (14) and (16) we have

$$\begin{aligned}
 [\mathbf{c}_i(\gamma) - \mathbf{c}_i(\boldsymbol{\eta})]_k &= \mathbf{v}_k^H [\mathbf{B}_n(v_i + \gamma_i/s_i) - \mathbf{B}_n(v_i + \eta_i/s_i)] \mathbf{u}_i \\
 &= (\eta_i - \gamma_i) \mathbf{v}_k^H r_n \mathbf{K}(v_i + \gamma_i/s_i - Q_n)^{-1} (v_i + \eta_i/s_i - Q_n)^{-1} Q_n p_n \mathbf{u}_i
 \end{aligned}$$

using (5).

Assuming $|v_i| > \frac{\|\gamma\|}{|s_i|} + \|Q_n\|$ for $\gamma \in D$ then there exists a constant β_1 independent of n such that

$$\|\mathbf{c}_i(\gamma) - \mathbf{c}_i(\boldsymbol{\eta})\| \leq \beta_1 \|Q_n p_n \mathbf{u}_i\| \|\gamma - \boldsymbol{\eta}\|.$$

Thus we take

$$C_1 = \beta_1 \|Q_n p_n \mathbf{u}_i\|. \tag{19}$$

Note: We shall introduce various quantities $\beta_i, i = 1, \dots, 6$, to make the analysis less complicated. In practical calculation they are replaced by specific expressions.

Also

$$\|\mathbf{c}_i(\mathbf{0})\| \leq \|\mathbf{B}_n(v_i) \mathbf{u}_i\| \tag{20}$$

and there is a constant β_2 say, independent of n , such that

$$H_0 = \|\mathbf{H}(\mathbf{0})\| \leq b \beta_2 \|\mathbf{B}_n(v_i)\| \tag{21}$$

where

$$b = \sum' |(v_i - v_j) s_j|^{-1}. \tag{22}$$

Finally

$$H_1 \leq b \beta_1 \|Q_n p_n\| \tag{23}$$

and

$$M_1 = \max_{j \neq i} |(v_i - v_j) s_i|^{-1} \neq 0 \quad \text{since } v_i \text{ is simple.} \tag{24}$$

If $g = \frac{2(M_1 + H_1) \|\mathbf{c}_i(\mathbf{0})\|}{(1 - C_1 - H_0)^2} < \frac{1}{2}$ then the result of the lemma gives

$$\|\gamma\| \leq \frac{\|\mathbf{B}_n(v_i) \mathbf{u}_i\|}{1 - \beta_1 \|Q_n p_n \mathbf{u}_i\| - n \beta_2 \|\mathbf{B}_n(v_i)\|} w(g).$$

If $n \|\mathbf{B}_n(v_i)\| \rightarrow 0$ as $n \rightarrow \infty$ then there is a bounded quantity β_3 such that

$$\|\gamma\| \leq \beta_3 \|\mathbf{B}_n(v_i) \mathbf{u}_i\|.$$

Using (14), (15) and (11) we obtain

$$|\lambda_i - v_i| \leq \beta_3 \frac{\|\mathbf{B}_n(v_i) \mathbf{u}_i\|}{|s_i|}, \tag{25}$$

$$|\alpha_{ik}| \leq \beta_3 \frac{\|\mathbf{B}_n(v_i) \mathbf{u}_i\|}{(v_i - v_j) s_j} \tag{26}$$

and

$$\|x_i - u_i\| \leq \beta_3 b \|B_n(v_i) u_i\|. \quad (27)$$

In fact (27) is unsatisfactory since b depends on n but we see later [Eq. (32)] that a more satisfactory expression for the rate of convergence can be obtained.

Finally in this section we obtain a bound for the rate of convergence of $p_n u$ to x .

$$\|x - p_n u\| \leq \|x - p_n x\| + \|p_n(x - u)\|. \quad (28)$$

Now from (2),

$$\lambda(1 - p_n r_n) x = (1 - p_n r_n) K x = (1 - p_n r_n) K p_n r_n x + (1 - p_n r_n) K(1 - p_n r_n) x.$$

If $|\lambda| > \|(1 - p_n r_n) K\| = \|Q_n\|$ then

$$(1 - p_n r_n) x = (\lambda - Q_n)^{-1} Q_n p_n x$$

and there is a bounded quantity β_4 such that

$$\|(1 - p_n r_n) x\| = \|x - p_n x\| \leq \beta_4 \|Q_n p_n x\|.$$

Thus, writing $x = (x - u) + u$ and using (28) there is a bounded quantity β_5 such that

$$\|x_i - p_n u_i\| \leq \beta_5 b \|B_n(v_i) u_i\|.$$

Computational experience indicates that if the kernel is smooth enough then for simple eigenvalues

$$|\lambda_i - v_i| = O(\text{error in quadrature rule}).$$

Clearly, from (27), to give a meaningful error analysis of the Nyström method we must choose p_n and r_n such that

$$\|B_n(v_i) u_i\| = O(\text{error in quadrature rule})$$

with $B_n(v_i)$ given by (5). In Section 4 this is discussed in detail for the trapezoidal rule. Briefly this can be done if $k(s, t)$ is smooth enough. If $k(s, t)$ is not smooth enough or even weakly singular then product integration should be used and a slightly different analysis is required. This is discussed briefly in Section 4 in [7] and in more detail in [8].

3. Dominant Error Terms and Their Estimation

Equation (18) also furnishes estimates of error and bounds for the estimates.

Write (28) as

$$\gamma - c_i(\mathbf{0}) = c_i(\gamma) - c_i(\mathbf{0}) + H(\gamma) \gamma + M(\gamma) \gamma.$$

Thus

$$\|\gamma - c_i(\mathbf{0})\| \leq C_1 \|\gamma\| + H_0 \|\gamma\| + H_1 \|\gamma\|^2 + M_1 \|\gamma\|^2$$

using (i) and (ii) of the lemma. The bounds (19)–(24) give

$$\|\boldsymbol{\gamma} - \mathbf{c}_i(\mathbf{0})\| \leq b \beta_6 \|\mathbf{B}_n(v_i) \mathbf{u}_i\|^2 \tag{29}$$

for some bounded constant β_6 .

Thus using (15) and (16) we obtain

$$\left| \alpha_{ik} - \frac{\mathbf{v}_k^H \mathbf{B}_n(v_i) \mathbf{u}_i}{(v_i - v_k) s_k} \right| \leq \frac{b \beta_6 \|\mathbf{B}_n(v_i) \mathbf{u}_i\|^2}{|(v_i - v_k) s_k|},$$

and, using (11) we obtain

$$\|\mathbf{x}_i - (\mathbf{u}_i + \mathbf{P}^{(i)} \mathbf{B}_n(v_i) \mathbf{u}_i)\| \leq b^2 \beta_6 \|\mathbf{B}_n(v_i) \mathbf{u}_i\|^2 \tag{30}$$

where

$$\mathbf{P}^{(i)} = \sum_{i \neq j} \frac{\mathbf{u}_i \mathbf{v}_j^H}{(v_i - v_j) s_j}. \tag{31}$$

Hence, using (10),

$$\|\mathbf{P}^{(i)}\| \leq \sum_{i \neq j} |(v_i - v_j) s_j|^{-1} = b \quad (\text{see (22)}).$$

It turns out that, for a simple eigenvalue v_i , even if $\|\mathbf{P}^{(i)}\|$ becomes unbounded as $n \rightarrow \infty$,

$$\|\mathbf{P}^{(i)} \mathbf{B}_n(v_i) \mathbf{u}_i\| = O(\|\mathbf{B}_n(v_i) \mathbf{u}_i\|) \quad (\text{see Table 2}).$$

Thus the term b in (29) and (30) is misleading. A better expression for the rate of convergence of \mathbf{u}_i to \mathbf{x}_i is

$$\|\mathbf{x}_i - \mathbf{u}_i\| = O(\|\mathbf{P}^{(i)} \mathbf{B}_n(v_i) \mathbf{u}_i\|). \tag{32}$$

Finally, it is straightforward to show using (29), (17), (14), and (16) that the dominant error term for the eigenvalue is given by

$$\left| \lambda_i - \left(v_i + \frac{\mathbf{v}_i^H \mathbf{B}_n(v_i) \mathbf{u}_i}{s_i} \right) \right| = O(\|\mathbf{P}^{(i)} \mathbf{B}_n(v_i) \mathbf{u}_i\| \cdot \|\mathbf{B}_n(v_i) \mathbf{u}_i\|). \tag{33}$$

Clearly it is difficult to calculate $\mathbf{B}_n(v_i) \mathbf{u}_i$ because of the term $(v_i - Q_n)^{-1}$ (see (5)). Let us define the matrix

$$G_n(v_i) = r_n K p_n - \mathbf{K}_n + \frac{1}{v_i} r_n K Q_n p_n. \tag{34}$$

Using the result

$$1/v_i - (v_i - Q_n)^{-1} = -\frac{1}{v_i} (v_i - Q_n)^{-1} Q_n$$

provided $|v_i| > \|Q_n\|$, we have

$$\|\mathbf{B}_n(v_i) \mathbf{u}_i - G_n(v_i) \mathbf{u}_i\| = O(\|Q_n^2 p_n \mathbf{u}_i\|). \tag{35}$$

Thus we shall estimate $\mathbf{B}_n(v_i) \mathbf{u}_i$ by $\mathbf{G}_n(v_i) \mathbf{u}_i$ in (30) and (33) and (35) implies that the rate of convergence will not be altered since $\|\mathbf{Q}_n p_n \mathbf{u}_i\| \leq \|\mathbf{B}_n(v_i) \mathbf{u}_i\|$.

The assumption at the beginning of Section 2 that \mathbf{K}_n has distinct eigenvalues can easily be overcome. The important requirement for the analysis of Section 2 is the existence of two sets of linearly independent eigenvectors $\{\mathbf{v}_i^H\}$, $\{\mathbf{u}_i\}$ satisfying $\mathbf{v}_i^H \mathbf{u}_j = s_i \delta_{ij}$. Assume that \mathbf{K}_n has a simple eigenvalue $v_i^{(n)}$ but that the other eigenvalues can be multiple. Clearly there is no difficulty if \mathbf{K}_n has a full set of linearly independent eigenvectors, however, if \mathbf{K}_n does not we can include generalised eigenvectors to produce two sets of vectors satisfying the required condition. An analysis similar to that in Section 2 follows. The dominant error term for $(\lambda_i - v_i)$ remains the same, but the expression for $\mathbf{x}_i - \mathbf{u}_i$ is altered, however, only by terms of order $\|\mathbf{B}_n(v_i) \mathbf{u}_i\|$. Thus the overall rate of convergence is not altered. Details of this approach can be found in [8].

4. p_n and r_n for the Trapezoidal Rule

Consider the numerical solution of (1) using the repeated trapezoidal rule. For a given n take $h = (b - a)/(n - 1)$; $w_i = h$, $i = 2, \dots, n - 1$; $w_1 = w_n = h/2$, $t_i = a + (i - 1)h$, $i = 1, \dots, n$.

Assume that $k(s, t) \in C^2[a, b] \times [a, b]$ and so the matrix in (3) has the form

$$(\mathbf{K}_n)_{ij} = w_j k(t_i, t_j).$$

The error in the repeated trapezoidal rule is $O(h^2)$ provided the integrand is smooth enough and so to give a satisfactory error analysis p_n and r_n must be chosen so that $\|\mathbf{B}_n(v_i)\| = O(h^2)$. This can be done under the above assumption on $k(s, t)$. Take

$$r_n x = [x(t_1), \dots, x(t_n)] \tag{36}$$

and

$$p_n \mathbf{u} = \sum_{j=1}^n \phi_j(t) u_j \tag{37}$$

where

$$\phi_j(t) = \begin{cases} 1 - \frac{|t - t_j|}{h} & t \in [t_{j-1}, t_{j+1}] \cap [a, b] \\ 0 & \text{elsewhere.} \end{cases} \tag{38}$$

$p_n \mathbf{u}$ is the piecewise linear function formed by joining the points (t_j, u_j) .

If $x \in C^2[a, b]$ then $p_n r_n x$ is the linear interpolating polynomial and

$$\|(1 - p_n r_n) x\| = \frac{h^2}{8} \|x''\|. \tag{39}$$

It is easy to show, using (39), that

$$\|Q_n\| = \|(1 - p_n r_n) K\| = \frac{h^2}{8} \|K_{ss}\| \tag{40}$$

where K_{ss} is the integral operator with kernel $\frac{\partial^2 k}{\partial s^2}(s, t)$.

To show that $\|r_n K p_n - K_n\| = O(h^2)$ consider

$$\begin{aligned} [r_n K p_n - K_n]_{ij} &= \int_a^b k(t_i, t) \phi_j(t) dt - w_j k(t_i, t_j) \\ &= \int_a^b \phi_j(t) [k(t_i, t) - k(t_i, t_j)] dt \end{aligned}$$

using the relation

$$w_j = \int_a^b \phi_j(t) dt.$$

It is easy to show

$$\|r_n K p_n - K_n\| \leq \frac{h^2}{6} \{ \|K_{tt}\| + \max(|k_t(s, a)| + |k_t(s, b)|) \}.$$

Clearly if $|v_i| > \frac{h^2}{8} \|K_{ss}\| = \|Q_n\|$ then (5) implies

$$\|B_n(v_i) u_i\| = O(h^2). \tag{41}$$

Thus the p_n and r_n defined by (36) and (37) are suitable for a satisfactory error analysis of the Trapezoidal rule. (In [8] p_n and r_n are found which allow a satisfactory analysis of the mid-point rule and Simpson’s rule methods. In [9] the Simpson’s rule method is discussed for equations of the second kind.)

Equations (25) and (32) with (41) show

$$|\lambda_i - v_i^{(n)}| = O(h^2) \tag{42}$$

and

$$\|x_i - u_i\| = O(h^2) \tag{43}$$

(see Tables 2 and 3).

Example. The integral Equation (1) with $k(s, t)$ given by

$$k(s, t) = s + \frac{3s}{6} (8s^3 - s) (t^3 - \frac{2}{3})$$

with $a=0, b=1$ has solutions

$$\begin{aligned} \lambda_1 &= 2 & x_1(s) &= s^3, \\ \lambda_2 &= 0.5 & x_2(s) &= s. \end{aligned}$$

Table 1

n	$v_1^{(n)} - \lambda_1$	Ratio	$\lambda_2 - v_2^{(n)}$	Ratio	$\ Q_n\ = \frac{h^2}{8} \ K_{ss}\ $
3	3.8995		-2.74444		2.538
		3.6		36.2	
5	1.0915		0.07573		0.634
		3.8		2.9	
9	0.2855		0.02602		0.159
		3.9		3.6	
17	0.0725		0.00728		0.040
		4.0		3.9	
33	0.0182		0.00188		0.010
		4.0		4.0	
65	0.0046		0.00047		0.003

The columns headed "Ratio" give the ratios of successive errors

The trapezium rule was used to provide numerical approximations. Table 1 supports (42) and also illustrates the importance of the condition $|\lambda| > \|Q_n\|$ [Eqs. (7) and (40)]. Now $\|Q_n\| > |\lambda_2| = 0.5$ for $n = 3, 5$ and we note that $O(h^2)$ convergence of $v_2^{(n)}$ to λ_2 is evident for $n = 17, 33, 65$. The approximations $v_1^{(n)}$ to λ_1 show $O(h^2)$ convergence for smaller n since $|\lambda_2| > \|Q_n\|$ for $n \geq 5$. Note that the absolute errors $\lambda_2 - v_2^{(n)}$ are smaller than the corresponding $\lambda_1 - v_1^{(n)}$ for $n \geq 5$. This is due to the greater smoothness of x_2 .

5. Calculation of $G_n(v_i) u_i$

As was mentioned at the end of Section 3 we replace $B_n(v_i) u_i$ in (30) and (33) by $G_n(v_i) u_i$ given by (34). We need to calculate $(r_n K p_n - K_n) u_i$ and $r_n K Q_n p_n u_i$. Let us assume that $k(s, t) \in C^4[s, t] \times [s, t]$.

For any $z \in E_n$

$$\begin{aligned}
 [r_n K p_n z]_j &= \int_a^b k(t_j, t) \sum_{p=1}^n \phi_p(t) z_p dt \\
 &= \sum_{i=1}^{n-1} \int_{t_i}^{t_{i+1}} k(t_j, t) [\phi_i(t) z_i + \phi_{i+1}(t) z_{i+1}] dt
 \end{aligned}$$

using (34).

Using Simpson's rule to evaluate the integrand over each subinterval we obtain, after rearrangement,

$$\begin{aligned}
 [r_n K p_n z]_j &= \frac{h}{6} [\{k(t_j, t_1) + 2k(t_j, t_{\frac{3}{2}})\} z_1 + \{2k(t_j, t_{n-\frac{3}{2}}) + k(t_j, t_n)\} z_n] \\
 &\quad + \frac{h}{3} \sum_{i=2}^{n-1} \{k(t_j, t_{i-\frac{3}{2}}) + k(t_j, t_i) + k(t_j, t_{i+\frac{3}{2}})\} z_i + O(h^4). \tag{44}
 \end{aligned}$$

Clearly $[(r_n K p_n - K_n) z]_j$ is easily calculated.

To estimate $r_n K Q_n p_n \mathbf{z} \equiv r_n K(1 - p_n r_n) K p_n \mathbf{z}$ we look firstly at $r_n K(1 - p_n r_n) f$ where $f \in C^4[a, b]$. Writing $f(t_p) = f_p$ we have

$$\begin{aligned}
 [r_n K(1 - p_n r_n) f]_j &= \sum_{i=1}^{n-1} \int_{t_i}^{t_{j+1}} k(t_j, t) \left(f(t) - \sum_{p=1}^n \phi_p(t) f_p \right) dt \\
 &= \frac{2h}{3} \sum_{i=1}^{n-1} k(t_j, t_{i+\frac{1}{2}}) [f_{i+\frac{1}{2}} - \frac{1}{2}(f_i + f_{i+1})] + O(h^4)
 \end{aligned}
 \tag{45}$$

again using Simpson’s rule over each subinterval. For $i=2, \dots, n-2$, we use

$$f_{i+\frac{1}{2}} - \frac{1}{2}(f_i + f_{i+1}) = \frac{1}{16}(-f_{i-1} + f_i + f_{i+1} - f_{i+2}) + O(h^4)$$

and for $i=1$,

$$f_{i+\frac{1}{2}} - \frac{1}{2}(f_i + f_{i+1}) = \frac{1}{16}(-3f_1 + 7f_2 - 5f_3 + f_4) + O(h^4)$$

with similar modification for $i=n-1$.

To estimate $[r_n K(1 - p_n r_n) K p_n \mathbf{z}]_j$ we use (45) with (44) giving the required quantities $[K p_n \mathbf{z}]_{s=t_i}$.

We suggested that $\|\mathbf{P}^{(1)} \mathbf{B}_n(v_i) \mathbf{u}_i\| = O(\|\mathbf{B}_n(v_i) \mathbf{u}_i\|)$ ($= O(h^2)$ for the trapezoidal rule).

This is confirmed by the results in Table 2. As h is halved, $\|\mathbf{P}^{(1)} \mathbf{B}_n(v_1^{(1)}) \mathbf{u}_1\|$ is quartered, even although $\|\mathbf{P}^{(1)}\|$ depends on n .

Table 2

n	$\ \mathbf{P}^{(1)} \mathbf{B}_n(v_1) \mathbf{u}_1\ $	$\ \mathbf{B}_n(v_1) \mathbf{u}_1\ $	$\ \mathbf{P}^{(1)}\ $
5	0.1939 E-1	0.2590	1.42
9	0.1325 E-1	0.4860 E-1	2.65
17	0.4738 E-2	0.1106 E-1	6.77
33	0.1310 E-2	0.2696 E-2	14.59
65	0.3361 E-3	0.6701 E-3	99.42

Equation (37) implies that $\left| \lambda_i - \left(v_i + \frac{\mathbf{v}_i^H \mathbf{B}_n(v_i) \mathbf{u}_i}{s_i} \right) \right| = O(h^4)$. Table 3 supports

this result. As h is halved the ratio of errors in successive corrected values is tending to 16 – an indication of $O(h^4)$ convergence.

Note that the correction produces a marked improvement in all cases even for small n .

Finally in this section we present the results for the estimation of the eigenvector. Clearly, from Table 4, $\|\mathbf{x}_1 - \mathbf{u}_1\| = O(h^2)$ and $\|\mathbf{x}_1 - (\mathbf{u}_1 + \mathbf{P}^{(1)} \mathbf{B}_n(v_1) \mathbf{u}_1)\| = O(h^4)$. The theoretical bounds (27) and (30) do not predict such a rapid rate of convergence (since b depends on n) but the presence of the b term is misleading and more detailed analysis gives (32) and

$$\|\mathbf{x}_1 - (\mathbf{u}_1 + \mathbf{P}^{(1)} \mathbf{B}_n(v_1) \mathbf{u}_1)\| = O(\|\mathbf{P}^{(1)} \mathbf{B}_n(v_1) \mathbf{u}_1\|^2).$$

These theoretical results agree with the computed results.

Table 3. The estimation of $\lambda_1=2$

n	$v_1^{(n)}$	$v_1^{(n)} + \text{correction}$	Ratio of errors in successive corrected values
5	3.09152	2.0293809	7.4
9	2.28545	2.0039899	12.3
17	2.07248	2.0003252	14.8
33	2.01820	2.0000219	15.6
65	2.00455	2.0000014	

Table 4. The estimation of $x_1(s)=s^3$

n	$\ \mathbf{x}_1 - \mathbf{u}_1\ _\infty$	Ratio	$\ \mathbf{x}_1 - (\mathbf{u}_1 + \mathbf{P}^{(1)} \mathbf{B}_n(v_1) \mathbf{u}_1)\ _\infty$	Ratio
5	0.18337 E-1	2.7	0.69082 E-2	6.5
9	0.69009 E-2	3.5	0.10621 E-3	11.5
17	0.19870 E-2	3.9	0.91958 E-4	14.6
33	0.51510 E-3	4.0	0.62885 E-5	15.6
65	0.13011 E-3		0.40269 E-6	

6. Numerical Performance of the Bounds of Section 3

Using the techniques of the previous section to estimate $\mathbf{G}_n(v_i) \mathbf{u}_i$ we can approximate the quantities C_1, H_0, H_1, M_1 and $\|\mathbf{c}_i(\mathbf{0})\|$ and hence estimate the bounds given in Section 2. The following results were obtained for the example at the end of Section 4.

Table 5

n	$\ \mathbf{c}_i(\mathbf{0})\ $	C_1	H_0	H_1	M_1	$\ \gamma\ $
5	0.259	0.357 E-2	1.45	0.113 E-1	1.54	(iii) of lemma violated
9	0.486 E-1	0.207 E-2	0.131	0.958 E-3	3.20	0.695 E-1
17	0.111 E-1	0.668 E-3	0.118	0.276 E-3	4.13	0.132 E-1
33	0.270 E-2	0.179 E-3	0.449 E-1	0.284 E-4	4.43	0.286 E-2
65	0.670 E-3	0.455 E-4	0.206 E-1	0.154 E-4	4.51	0.676 E-3

Table 6

n	True error = $ \lambda_1 - v_1^{(n)} $	Bound from (25)
5	1.092	(iii) of lemma violated
9	0.285	0.402
17	0.725 E-1	0.860 E-1
33	0.182 E-1	0.193 E-1
65	0.456 E-2	0.459 E-2

These results show that M_1 is approximately constant, H_0 and H_1 show $O(h)$ convergence, and $\|\mathbf{c}_i(\mathbf{0})\|$, C_1 , $\|\gamma\|$ show $O(h^2)$ convergence. This is in agreement with the theoretical results in Section 2. The numerical performance of the bound (25) is illustrated in the Table 6.

Clearly the bounds obtained for this example are very good. Asymptotically we have

$$|\lambda - v_i^{(n)}| \leq (1 + o(n^{-1})) \max_k |v_k^H \mathbf{B}_n(v_i) \mathbf{u}_i| / s_i.$$

If the maximum occurs for $k = i$ then the bound becomes

$$|\lambda_i - v_i^{(n)}| \leq (1 + o(n^{-1})) \text{ (the dominant error term given by (33))}.$$

This is the case in the above example.

In this paper the bounds are calculated as accurately as possible. For example we calculate $\|\mathbf{c}_i(\mathbf{0})\|$ in Table 5 from $\|\mathbf{c}_i(\mathbf{0})\| = \max_k |v_k^H \mathbf{B}_n(v_i) \mathbf{u}_i|$ instead of $\|\mathbf{c}_i(\mathbf{0})\| \leq \|\mathbf{B}_n(v_i) \mathbf{u}_i\|$. The latter is cheaper of course but less sharp. However the bounds are expensive to calculate. In particular all the eigenvalues with their corresponding left and right eigenvectors have to be found. Also we have to calculate the matrix with (p, q) -th component $v_p^H \mathbf{G}_n(v_i) \mathbf{u}_q$ [see (34)], i.e.

$$X_{pq} + \frac{1}{v_i} Y_{pq} \quad \text{with} \quad X_{pq} = v_p^H (r_n K_n p_n - \mathbf{K}_n) \mathbf{u}_q$$

$$\text{and} \quad Y_{pq} = v_p^H r_n K (1 - p_n r_n) K p_n \mathbf{u}_q.$$

This is very expensive. However once X_{pq} and Y_{pq} are calculated they can be used to provide bounds and estimates for all the simple eigenvalues and eigenvectors (provided the conditions of the lemma hold). If bounds are required for several eigenvalues and eigenvectors then we would be justified in doing the work. If we are interested in only one eigenvalue then the bounds would probably be too expensive to calculate. Note however that the estimate of the error given by (33) requires only the calculation of v_i and s_i .

The eigenvalues and right eigenvectors are calculated using QR as described in [13, contributions II/14 and II/15]. The left eigenvectors are found by calculating the left eigenvectors of the 2×2 block triangular matrix obtained in QR and transforming in the usual manner. Note that if $k(s, t)$ is symmetric then we can solve a symmetric eigenvalue problem and the left eigenvectors are identically the right eigenvectors.

We give below the timings for various stages in the calculation of the estimates and bounds. We define the times T_i $i = 1, \dots, 5$ as follows.

Table 7

n	T_1	T_2	T_3	T_4	T_5
5	0.06	0.04	0.05	0.002	—
9	0.43	0.29	0.33	0.006	0.008
17	2.70	1.85	2.12	0.019	0.027
33	15.19	10.71	14.67	0.069	0.101
65	104.45	74.75	116.80	0.260	0.385

The times are given in seconds on the ICL System 4-70 at University College, Cardiff, Wales

T_1 = time to calculate $v_i^{(n)}, u_i \ i = 1, \dots, n$,

T_2 = time to calculate the left eigenvectors $v_i \ i = 1, \dots, n$,

T_3 = time to calculate $v_p^H G_n(v_i) u_q \ p, q = 1, \dots, n$,

T_4 = time to calculate estimates (33) and (30) appearing in Tables 3 and 4,

T_5 = time to calculate bounds in Tables 5 and 6.

The calculation of the n^2 elements $v_p^H G_n(v_i) u_q$ takes about the same time as the solution of the eigenvalue problem. Once these have been calculated estimates and bounds are easily obtained.

7. Concluding Remarks

In this paper rigorous error bounds and dominant error terms have been obtained for approximations to the solutions of (1) obtained using the Nyström method. In Sections 5 and 6 it was demonstrated how these bounds and estimates may be calculated. In all cases considered in [8] the addition of the correction terms shown in (30) and (33) produced a significant improvement of the original approximation.

Finally we note that the dominant term in the correction of the eigenvalue, given by (33), is almost that given by the Rayleigh quotient approach. If we regard u_i as an approximation to x_i then the Rayleigh quotient correction for the eigenvalue is

$$v_i^H [K_n + B_n(\lambda)] u_i / s_i = v_i^{(n)} + \frac{v_i^H B_n(\lambda) u_i}{s_i}.$$

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