Error Reduction in Gauss-Jacobi-Nyström Quadrature for Fredholm Integral Equations of the Second Kind

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Abstract: A method is presented for improving the accuracy of the widely used Gauss-Legendre Nyström method for determining approximate solutions of Fredholm integral equations of the second kind on finite intervals. The authors' recent continuous-kernel approach is generalised in order to accommodate kernels that are either singular or of limited continuous differentiability at a finite number of points within the interval of integration. This is achieved by developing a Gauss-Jacobi Nyström method that moreover includes a mean-value estimate of the truncation error of the Hermite interpolation on which the quadrature rule is based, making it particularly accurate at low orders. A theoretical framework of the new technique is developed, implemented and validated on test problems with known exact solutions, and degenerate cases of the new Gauss-Jacobi scheme are corroborated against standard Gauss-Legendre and first- and second-kind Gauss-Chebyshev methods (i.e. using tabulated weights and abscissae). Significant error reductions over standard methods are observed, and all results are explained in the context of the new theory.

Keywords: Fredholm integral equations, Nyström method, numerical quadrature, Gauss-Jacobi polynomials, error analysis.

1 Introduction

This paper extends the authors' recent method (Kelmanson and Tenwick (2009)) for improving the accuracy of the well-known Gauss-Legendre Nyström method (Nyström (1930)) for determining approximate solutions of Fredholm integral equations of the second kind (FIE2s) on finite intervals, in the case when the kernel of the FIE2 is infinitely continuously differentiable. If, however, the kernel is either singular or of limited continuous differentiability within the interval of integration, a more general approach—one based upon Gauss-Jacobi quadrature, of which

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Gauss-Legendre is a special case—is necessary. Development of such an approach constitutes the present work.

We consider the FIE2 for the unknown function $U(T)$ on the finite interval $[a, b]$, with kernel $\widetilde{K}(T, S)$ and source term $F(T)$,

$$U(T) - \Lambda \int_a^b \widetilde{K}(T, S) U(S) \, dS = F(T); \qquad T \in [a, b], \tag{1}$$

in which Λ is a real constant. Without loss of generality we assume that $\widetilde{K}(T, S)$ is infinitely continuously differentiable with respect to S for all interior $S \in (a, b)$; if $\widetilde{K}(T, S)$ is either singular or finitely continuously differentiable at a finite number, m say, of points $\{S_i\}_{i=1}^m \in (a, b)$, a modification of the theory and implementation in this paper should be applied over the union of sub-intervals $\cup_{i=1}^{m-1}[S_i, S_{i+1}] \cup [a, S_1] \cup [S_m, b]$.

To admit the possibility that $\widetilde{K}(T, S)$ has either end-point singularities or limited end-point differentiability, the kernel in Eq. 1 is factorised as

$$U(T) - \Lambda \int_a^b (b - S)^\mu (S - a)^\nu K(T, S) U(S) \, dS = F(T) \qquad T \in [a, b], \tag{2}$$

in which $K(T, S)$ is infinitely differentiable with respect to S, and μ and ν are parameters with $\mu, \nu > -1$, so that Eq. 2 may be singular but not hypersingular. Via the linear transformation

$$(T, S) = \frac{b - a}{2}(t, s) + \frac{b + a}{2}(1, 1), \tag{3}$$

Eq. 2 transforms into the canonical form

$$u(t) - \lambda \int_{-1}^1 (1 - s)^\mu (1 + s)^\nu k(t, s) u(s) \, ds = f(t), \qquad t \in [-1, 1], \tag{4}$$

in which lower-case functions and variables on $[-1, 1]$ correspond to their upper-case counterparts on $[a, b]$ in Eq. 2 and $\lambda = \Lambda[(b - a)/2]^{\mu+\nu+1}$. We assume that λ is a regular value of Eq. 4, to which a unique solution $u(t)$ exists for $t \in [-1, 1]$. Defining the integral operator $\mathscr{K}$ (whose dependence on μ and ν is notationally suppressed for convenience) by

$$(\mathscr{K} u)(t) \equiv \int_{-1}^1 (1 - s)^\mu (1 + s)^\nu k(t, s) u(s) \, ds, \tag{5}$$

Eq. 4 may be written in symbolic form as

$$u - \lambda \mathscr{K} u = f, \tag{6}$$

with unique solution given by

$$u = (\mathscr{I} - \lambda \mathscr{K})^{-1} f, \tag{7}$$

in which $\mathscr{I}$ is the identity operator and, from which, by implication,

$$||(\mathscr{I} - \lambda \mathscr{K})^{-1}|| < \infty. \tag{8}$$

Despite the symbolic implication of Eq. 7, an explicit closed-form continuous solution $u(t)$ of Eq. 4 cannot in general be obtained for an arbitrary kernel factor $k(t,s)$, and many numerical quadrature and projection schemes for determining approximate solutions $u_n(t)$, either piecewise or globally interpolated through $n \in \mathbb{N}$ discrete nodal values in $[-1, 1]$, are thoroughly addressed in, e.g., Atkinson (1997); Baker (1977); Delves and Mohamed (1985); Hackbusch (1989); Kress (1999); Mason and Handscomb (2003). Of all such methods, we presently focus on the (global) Nyström method (Nyström (1930)), which continues to be the subject of new developments and applications on diverse fronts (e.g. Benko, Biles, Robinson, and Spraker (2008); Dick, Kritzer, Kuo, and Sloan (2007); Kang, Koltracht, and Rawitscher (2002); Mastroianni and Monegato (2003)). In the notation of Eq. 6, the symbolic form of the Nyström method for finding the approximation u_n to u is

$$u_n - \lambda \mathscr{K}_n u_n = f, \tag{9}$$

in which specification of the explicit form of the quadrature rule $\mathscr{K}_n u_n$ is deferred until §2, and in which the occurrence of f, rather than an approximation f_n, on the right-hand side reflects the quadrature, rather than projection, nature of the approximation. From Eq. 6 and Eq. 9, the Nyström error satisfies

$$u - u_n = \lambda (\mathscr{I} - \lambda \mathscr{K}_n)^{-1} (\mathscr{K} - \mathscr{K}_n) u, \tag{10}$$

in which the inverse operator exists and, by Eq. 8 and Theorem 4.1.2 in Atkinson (1997), is bounded according to

$$||(\mathscr{I} - \lambda \mathscr{K}_n)^{-1}|| \leq \frac{1 + |\lambda| \, ||(\mathscr{I} - \lambda \mathscr{K})^{-1}|| \, ||\mathscr{K}_n||}{1 - \lambda^2 ||(\mathscr{I} - \lambda \mathscr{K})^{-1}|| \, ||(\mathscr{K} - \mathscr{K}_n) \mathscr{K}_n||},$$

provided that

$$||(\mathscr{K} - \mathscr{K}_n) \mathscr{K}_n|| < \frac{1}{\lambda^2 \, ||(\mathscr{I} - \lambda \mathscr{K})^{-1}||} : \tag{11}$$

by Eq. 4.1.19 in Atkinson (1997), this is true for sufficiently large n. Taking bounds in Eq. 10, the Nyström error therefore satisfies

$$||u - u_n||_\infty \leq \xi_n \, ||(\mathscr{K} - \mathscr{K}_n) u||_\infty \tag{12}$$

for some finite positive constant ξ_n and sufficiently large n. Hence the Nyström error converges to zero with n at the same rate as that of the error of the quadrature implicit in Eq. 9 so, by using rules based on suitable orthogonal polynomials, one may obtain spectral convergence of $||u-u_n||_\infty$ with n uniformly throughout $[-1,1]$. For example, and notwithstanding the recent observations in Trefethen (2008), it can be shown (see derivation of Eq. 55) that, if Gauss-Jacobi quadrature is used in Eq. 4 to compute $\mathscr{K}_n u_n$ in Eq. 9, the large-n asymptotic estimate of the Gauss-Jacobi Nyström error bound[1] is

$$||u-u_n||_\infty \leq \frac{\pi}{2^{2n+\mu+\nu}(2n)!}\,||\partial_{2n}[k(t,s)\,u(s)]||_\infty, \qquad n \to \infty, \tag{13}$$

in which ∂_m denotes m-fold differentiation with respect to s. Hence, since the kernel factor $k(t,s)$ in Eq. 2 is by construction infinitely continuously differentiable with respect to s, Eq. 13 reveals that $||u-u_n||_\infty$ converges to zero exponentially with n when $\partial_{2n}u(s)$ is bounded.

Effective methods (for solving Eq. 4) based on Chebyshev-polynomial interpolation of $u(t)$ are presented in Brutman (1993) and Mason and Handscomb (2003), the former of which is similar to the forced-oscillation near-minimax approximation of p.232 *et seq.* in Atkinson (1989); such methods enjoy the property of yielding accurate estimates of approximation errors $||u-u_n||_\infty$ that are moreover, by the Chebyshev equioscillation theorem, near-uniform throughout the interval $[-1,1]$.

The aim of this paper is to modify the standard orthogonal-polynomial Nyström method in order to reduce $||u-u_n||_\infty$ for a given *low value* of n. In §2 the general theoretical framework underlying the modified method is presented and, in §3, the details of its finite-dimensional implementation are given. Finally, in §4 the new method is applied to several examples using Gauss-Jacobi quadrature, of which Gauss-Legendre and Gauss-Chebyshev (first and second kind) quadratures are special cases; all results are interpreted in the context of the theory of §2.

2 Theory

Since the Jacobi polynomials $P_n^{(\mu,\nu)}(s)$ are orthogonal on $s \in [-1,1]$ with respect to the weight function in the integral in Eq. 4,

$$\int_{-1}^{1}(1-s)^\mu\,(1+s)^\nu\,P_i^{(\mu,\nu)}(s)\,P_j^{(\mu,\nu)}(s)\,ds = \delta_{ij}, \qquad i,j \in \mathbb{N}, \tag{14}$$

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[1] When $\mu = \nu = 0$, Gauss-Jacobi quadrature reduces to Gauss-Legendre quadrature, whence Eq. 13 agrees with the asymptotic estimate of Eq. 5.3.37 in Atkinson (1989).

the explicit form of the orthogonal-polynomial quadrature approximation of $\mathscr{K}u$ in Eq. 10 is

$$(\mathscr{K}_n u)(t) \equiv \sum_j c_{j,n} k(t, \sigma_j) u(\sigma_j), \qquad t \in [-1, 1], \tag{15}$$

in which the quadrature weights are given by (see, e.g., Gautschi (2004))

$$c_{j,n} = -\frac{A_{n+1}\, \gamma_n}{A_n\, P_{n+1}^{(\mu,\nu)}(\sigma_j)\, \partial_1 P_n^{(\mu,\nu)}(\sigma_j)}, \tag{16}$$

where

$$A_n = \frac{(2n + \mu + \nu)!}{2^n\, n!\, (n + \mu + \nu)!} \tag{17}$$

is the coefficient of s^n in $P_n^{(\mu,\nu)}(s)$, the nodes (abscissae) σ_j are the n distinct roots of $P_n^{(\mu,\nu)}(s) = 0$, and γ_n is given by

$$\gamma_n = \int_{-1}^{1} (1-s)^\mu\, (1+s)^\nu\, \left[P_n^{(\mu,\nu)}(s)\right]^2 ds, \tag{18}$$

evaluation of which (Abramowitz and Stegun (1972), §22.1) yields the quadrature weights of Eq. 16 in the explicit computable form

$$c_{j,n} = \frac{2^{\mu+\nu}\, (2n + \mu + \nu + 2)\, \Gamma(n + \mu + 1)\, \Gamma(n + \nu + 1)}{\Gamma(n+2)\, \Gamma(n + \mu + \nu + 2)\, P_{n+1}^{(\mu,\nu)}(\sigma_j)\, \partial_1 P_n^{(\mu,\nu)}(\sigma_j)}. \tag{19}$$

If u is sufficiently differentiable (see Eq. 56), the quadrature error defined by

$$(\mathscr{E}_n u)(t) \equiv ((\mathscr{K} - \mathscr{K}_n)u)(t) \tag{20}$$

is pointwise convergent,

$$(\mathscr{E}_n u)(t) \to 0, \qquad n \to \infty, \qquad t \in [-1, 1], \tag{21}$$

but not norm convergent (Hackbusch (1989), Lemma 4.7.6),

$$||\mathscr{E}_n|| \geq ||\mathscr{K}||, \qquad \forall n \in \mathbb{N}. \tag{22}$$

However, if $\widetilde{\mathscr{E}}_n u$ is an approximation of the true quadrature error $\mathscr{E}_n u$, the *error discrepancy* defined by

$$(\Delta \widetilde{\mathscr{E}}_n u)(t) \equiv ((\widetilde{\mathscr{E}}_n - \mathscr{E}_n)u)(t), \tag{23}$$

must, by construction, satisfy

$$||\Delta \widetilde{\mathscr{E}}_n|| \to 0, \qquad n \to \infty \tag{24}$$

from which, additionally (Atkinson (1997), Eq. 4.1.19),

$$||\widetilde{\mathscr{E}}_n \mathscr{K}_n|| \to 0, \qquad n \to \infty. \tag{25}$$

The modified Nyström method, with solution $\bar{u}_n$, is based upon augmenting the standard Nyström method of Eq. 9 with the approximation $\widetilde{\mathscr{E}}_n \bar{u}_n$ of the true quadrature error $\mathscr{E}_n \bar{u}_n$,

$$\bar{u}_n - \lambda \left(\mathscr{K}_n \bar{u}_n + \widetilde{\mathscr{E}}_n \bar{u}_n \right) = f, \tag{26}$$

equivalently

$$(\mathscr{I} - \lambda \mathscr{K}_n - \lambda \widetilde{\mathscr{E}}_n) \bar{u}_n = f, \tag{27}$$

which, by Eq. 20 and Eq. 23, is moreover equivalent to

$$(\mathscr{I} - \lambda \mathscr{K} - \lambda \Delta \widetilde{\mathscr{E}}_n) \bar{u}_n = f. \tag{28}$$

Hence the *modified Nyström operator* $\mathscr{I} - \lambda \mathscr{K}_n - \lambda \widetilde{\mathscr{E}}_n$ in Eq. 27 is invertible if and only if $\mathscr{I} - \lambda \mathscr{K} - \lambda \Delta \widetilde{\mathscr{E}}_n$ in Eq. 28 is invertible. To prove this, consider the identity

$$(\mathscr{I} - \lambda \mathscr{K} - \lambda \Delta \widetilde{\mathscr{E}}_n)^{-1} = \left[\mathscr{I} - \lambda (\mathscr{I} - \lambda \mathscr{K})^{-1} \Delta \widetilde{\mathscr{E}}_n \right]^{-1} (\mathscr{I} - \lambda \mathscr{K})^{-1}, \tag{29}$$

in which, by Eq. 8, the second inverse on the right-hand side is bounded. Hence, defining

$$\mathscr{A}_n \equiv \lambda (\mathscr{I} - \lambda \mathscr{K})^{-1} \Delta \widetilde{\mathscr{E}}_n, \tag{30}$$

the limit in Eq. 24 reveals that there exists an $N \in \mathbb{N}$ such that

$$||\mathscr{A}_n|| = |\lambda| \, ||(\mathscr{I} - \lambda \mathscr{K})^{-1}|| \, ||\Delta \widetilde{\mathscr{E}}_n|| < 1, \qquad n \geq N,$$

whence the geometric series theorem gives both the bound

$$||(\mathscr{I} - \mathscr{A}_n)^{-1}|| \leq \frac{1}{1 - ||\mathscr{A}_n||} \tag{31}$$

and the explicit form of the inverse as the Neumann series

$$(\mathscr{I} - \mathscr{A}_n)^{-1} = \sum_{j=0}^{\infty} \mathscr{A}_n^j. \tag{32}$$

Thus, when condition Eq. 24 is satisfied, the modified Nyström operator in Eq. 27 has a bounded inverse by Eq. 29–Eq. 32, whence a unique solution $\bar{u}_n$ can be obtained.

Via Eq. 20, the standard Nyström error of Eq. 10 satisfies

$$(\mathscr{I} - \lambda \mathscr{K}_n)(u - u_n) = \lambda \mathscr{E}_n u, \tag{33}$$

whereas Eq. 27 can be used to show that the modified Nyström error satisfies

$$(\mathscr{I} - \lambda \mathscr{K}_n - \lambda \widetilde{\mathscr{E}}_n)(u - \bar{u}_n) = \lambda \Delta \widetilde{\mathscr{E}}_n u. \tag{34}$$

Accordingly, Eq. 34 and Eq. 31 yield the error bound

$$||u - \bar{u}_n||_\infty \leq \zeta_n ||\Delta \widetilde{\mathscr{E}}_n u||_\infty, \tag{35}$$

for some finite positive constant ζ_n and sufficiently large n. However, using Eq. 20 to rewrite Eq. 12 as

$$||u - u_n||_\infty \leq \xi_n ||\widetilde{\mathscr{E}}_n u||_\infty, \tag{36}$$

it is evident that the standard and modified Nyström error bounds are respectively proportional to an error and an error discrepancy, whence the essence of the new method is expressed as

$$||u - \bar{u}_n||_\infty \ll ||u - u_n||_\infty. \tag{37}$$

As shown in §3, $\widetilde{\mathscr{E}}_n$ is a differential operator, direct action of which on the numerical solution $\bar{u}_n$ in Eq. 26 necessitates high-order differentiation (at an accuracy consistent with that of Nyström integration) of irregularly spaced nodal values, which spacing moreover varies with n. To avert this potentially complex numerical differentiation, Eq. 26 is written as an implicit equation for $\bar{u}_n$,

$$\bar{u}_n = f + \lambda (\mathscr{K}_n \bar{u}_n + \widetilde{\mathscr{E}}_n \bar{u}_n), \tag{38}$$

which can be used recursively to replace $\bar{u}_n$ wherever it occurs as the direct operand of (a positive integer power of) $\widetilde{\mathscr{E}}_n$. Applying $M \geq 1$ such recursive iterations, Eq. 38 yields

$$\bar{u}_n = \sum_{m=0}^{M} (\lambda \widetilde{\mathscr{E}}_n)^m f + \lambda \sum_{m=0}^{M} (\lambda \widetilde{\mathscr{E}}_n)^m \mathscr{K}_n \bar{u}_n + (\lambda \widetilde{\mathscr{E}}_n)^{M+1} \bar{u}_n. \tag{39}$$

Defining the linear operator $\widetilde{\mathscr{E}}_n^{(\lambda, M)}$ by

$$\widetilde{\mathscr{E}}_n^{(\lambda, M)} \equiv \sum_{m=1}^{M} (\lambda \widetilde{\mathscr{E}}_n)^m \tag{40}$$

then, without error, Eq. 39 may be rewritten as

$$(\mathscr{I} - \lambda\,\mathscr{K}_n - \lambda\,\widetilde{\mathscr{E}}_n^{(\lambda,M)}\,\mathscr{K}_n - \lambda^{M+1}\,\widetilde{\mathscr{E}}_n^{M+1})\bar{u}_n^{(M)} = f + \widetilde{\mathscr{E}}_n^{(\lambda,M)}f, \tag{41}$$

in which $\bar{u}_n$ has been replaced by $\bar{u}_n^{(M)}$ to highlight the dependence upon M of its solution. In order to implement Eq. 41, the term $\lambda^{M+1}\,\widetilde{\mathscr{E}}_n^{M+1}$ must be neglected, which requires

$$||\lambda^{M+1}\,\widetilde{\mathscr{E}}_n^{M+1}|| \ll ||\mathscr{I} - \lambda\,\mathscr{K}_n - \lambda\,\widetilde{\mathscr{E}}_n^{(\lambda,M)}\,\mathscr{K}_n|| \le ||\mathscr{I} - \lambda\,\mathscr{K}_n|| + |\lambda|\,||\widetilde{\mathscr{E}}_n^{(\lambda,M)}\,\mathscr{K}_n||$$

so that, by Eq. 25 and Eq. 40, the *truncation condition* is

$$||\widetilde{\mathscr{E}}_n^{M+1}|| \ll \frac{||\mathscr{I} - \lambda\,\mathscr{K}_n||}{|\lambda|^{M+1}}, \qquad n \to \infty, \tag{42}$$

from which it is clear that the bound becomes more stringent with increasing M when $|\lambda| > 1$. When condition Eq. 42 holds, Eq. 41 can be approximated by the truncated equation that forms the theoretical basis of the new method,

$$(\mathscr{I} - \lambda\,\mathscr{K}_n - \lambda\,\widetilde{\mathscr{E}}_n^{(\lambda,M)}\,\mathscr{K}_n)\bar{u}_n^{(M)} = f + \widetilde{\mathscr{E}}_n^{(\lambda,M)}f, \tag{43}$$

in which all terms can be computed because all powers $(\widetilde{\mathscr{E}}_n)^m$ in $\widetilde{\mathscr{E}}_n^{(\lambda,M)}$ act upon the quadrature $\mathscr{K}_n\bar{u}_n^{(M)}$ rather than $\bar{u}_n^{(M)}$ directly; their action upon f is similarly computable. If we further define $\bar{u}_n^{(0)} \equiv \bar{u}_n$ and $\widetilde{\mathscr{E}}_n^{(\lambda,0)} \equiv 0$, the standard Nyström method of Eq. 9 is recovered by setting $M = 0$ in Eq. 43.

3   Implementation

The conditions are now determined under which the finite-dimensional representation of Eq. 43 is solvable. Recall that nodal values of u_n in the standard Nyström method are obtained by collocating a finite-dimensional approximation of Eq. 9 at each zero $t = \sigma_i$ of the Legendre polynomial $P_n(t)$, thereby generating a system of n linear equations for the components $u_n(\sigma_j)$ of the n-vector $\boldsymbol{u_n}$,

$$(\boldsymbol{I} - \lambda\,\boldsymbol{K})\,\boldsymbol{u_n} = \boldsymbol{f}, \tag{44}$$

in which $\boldsymbol{I}$ is the $n \times n$ identity matrix and the components of $\boldsymbol{K}$ and $\boldsymbol{f}$ are respectively $K_{i,j} = c_{j,n}k(\sigma_i,\sigma_j)$ and $f_i = f(\sigma_i)$. By Eq. 4.1.53 in Atkinson (1997), the system matrix in Eq. 44 satisfies

$$||(\boldsymbol{I} - \lambda\,\boldsymbol{K})^{-1}||_\infty \le ||(\mathscr{I} - \lambda\,\mathscr{K}_n)^{-1}||, \tag{45}$$

the right-hand side of which is bounded by Eq. 8. Hence the matrix $\boldsymbol{I} - \lambda\,\boldsymbol{K}$ in Eq. 44 is invertible. By analogy with Eq. 44, the nodes in the new modified method

are the zeros of the Jacobi polynomial $P_n^{(\mu,\nu)}(t)$, and the vector $\overline{\boldsymbol{u}}_{\boldsymbol{n}}^{(M)}$ of nodal values of $\overline{u}_n^{(M)}$ in the modified Nyström method of Eq. 43 satisfies the linear system

$$(\boldsymbol{I} - \lambda\,\boldsymbol{K} - \lambda\,\widetilde{\mathscr{E}}_n^{(\lambda,M)}\boldsymbol{K})\,\overline{\boldsymbol{u}}_{\boldsymbol{n}}^{(M)} = \boldsymbol{f} + \widetilde{\mathscr{E}}_n^{(\lambda,M)}\boldsymbol{f}\,, \tag{46}$$

in which detailed discussion of the components $(\widetilde{\mathscr{E}}_n^{(\lambda,M)}\boldsymbol{K})_{ij}$ and $(\widetilde{\mathscr{E}}_n^{(\lambda,M)}\boldsymbol{f})_i$ is by necessity deferred until an explicit form is given to $\widetilde{\mathscr{E}}_n$, which must display pointwise convergence,

$$(\widetilde{\mathscr{E}}_n u)(t) \to 0\,, \qquad n \to \infty\,, \qquad t \in [-1,1]\,, \tag{47}$$

in keeping with Eq. 21. Then, the linear operator $\widetilde{\mathscr{E}}_n^{(\lambda,M)}$ acting on the arbitrary matrix $\boldsymbol{A} = A_{i,j}$ yields a matrix with elements

$$\sum_{m=1}^{M} \lambda^m\, \widetilde{\mathscr{E}}_n^m\, A_{i,j}$$

which, by Eq. 47, satisfies $\widetilde{\mathscr{E}}_n^{(\lambda,M)}\boldsymbol{A} \to \boldsymbol{0}$ as $n \to \infty$, so that

$$||\,\widetilde{\mathscr{E}}_n^{(\lambda,M)}\boldsymbol{A}\,||_\infty \to 0\,, \qquad n \to \infty \tag{48}$$

for all $\boldsymbol{A}$ (with sufficiently differentiable elements). Since $\boldsymbol{I} - \lambda\,\boldsymbol{K}$ in Eq. 44 is invertible by Eq. 45, so is the matrix in Eq. 46 provided that (Golub and van Loan (1989), Theorem 2.3.4)

$$||\,\lambda\,(\boldsymbol{I} - \lambda\,\boldsymbol{K})^{-1}\,\widetilde{\mathscr{E}}_n^{(\lambda,M)}\boldsymbol{K}\,||_\infty < 1\,. \tag{49}$$

Hence, by standard norm inequalities and Eq. 49, we require

$$|\lambda|\,||\,(\boldsymbol{I} - \lambda\,\boldsymbol{K})^{-1}\,||_\infty\,||\,\widetilde{\mathscr{E}}_n^{(\lambda,M)}\boldsymbol{K}\,||_\infty < 1\,, \tag{50}$$

from which inversion of Eq. 46 is guaranteed by Eq. 48 for sufficiently large n (*cf.* Groh and Kelmanson (2008), Eq. (30)) . Thus, when the original Nyström system in Eq. 44 has a unique solution, so does the perturbed system in Eq. 46 for sufficiently large n.

The implementation is concluded by finding a computable error estimate $\widetilde{\mathscr{E}}_n$. The explicit form of $(\mathscr{E}_n u)(t)$ associated with the orthogonal-polynomial quadrature rule is

$$(\mathscr{E}_n^* u)(t,s^*) = \beta_n\,\delta_n^*(u;t,s^*)\,, \tag{51}$$

in which, by a natural extension of standard results (see, e.g., Gautschi (2004)),

$$\beta_n = \frac{\gamma_n}{A_n^2\,(2n)!} \qquad \text{and} \qquad \delta_n^*(u;t,s^*) = \{\partial_{2n}[k(t,s)\,u(s)]\}_{s=s^*}\,, \tag{52}$$

where $s^* \in [-1,1]$ is an unspecified parameter born of the mean-value form of the error of the Hermite interpolating polynomial from which Eq. 15–Eq. 19 are derived. From Eq. 17, Eq. 18 and Eq. 52 we compute, without error,

$$\beta_n = \frac{2^{\mu+\nu+1}\sqrt{\pi}\,\Gamma(n+\mu+1)\,\Gamma(n+\nu+1)\,\Gamma(n+\mu+\nu+1)}{\Gamma\left(n+\frac{1}{2}\right)\Gamma(2n+\mu+\nu+1)\,\Gamma(2n+\mu+\nu+2)}, \tag{53}$$

which readily yields the asymptotic ratio

$$\frac{\beta_{n+1}}{\beta_n} \sim \frac{1}{16n^2} - \frac{3}{32n^3} + \frac{4-\mu^2-\nu^2}{32n^4} + O(n^{-5}), \qquad n \to \infty, \tag{54}$$

so that β_n converges to zero exponentially with n independently of $\mu, \nu > -1$; this property is used in explaining features of the results in §4. A rather more complicated manipulation of Eq. 53 yields the asymptotic formula

$$\beta_n \sim \frac{\pi}{2^{2n+\mu+\nu}\,(2n)!}\left(1 + \frac{2\mu^2+2\nu^2-1}{4n} + O(n^{-2})\right), \qquad n \to \infty \tag{55}$$

which, irrespective of $\mu, \nu > -1$, is unexpectedly accurate for low values of n. For example, for $\mu = \nu = 0$ (when $P_n^{(\mu,\nu)}(s) = P_n(s)$, the Legendre polynomial of the first kind), the two-term asymptotic series for β_n in Eq. 55 is in error from the true value in Eq. 53 by only 3.36%, 1.57% and 0.91% for n as low as 2, 3 and 4 respectively. Moreover, for both $\mu = \nu = -\frac{1}{2}$ (when $P_n^{(\mu,\nu)}(s) = T_n(s)$, the Chebyshev polynomial of the first kind) and $\mu = \nu = \frac{1}{2}$ (when $P_n^{(\mu,\nu)}(s) = U_n(s)$, the Chebyshev polynomial of the second kind), the coefficient of every inverse power of n in the parenthetical series in Eq. 55 vanishes so that, without error,

$$\beta_n = \frac{\pi}{2^{2n\pm 1}\,(2n)!}, \qquad \mu = \nu = \pm\frac{1}{2}, \qquad \text{all } n \in \mathbb{N}.$$

Finally, the dependence in Eq. 51 of $\delta_n^*(u;t,s^*)$ upon the unknown s^* is circumvented by approximating it, with error ε_n^*, by its mean-value, integrated over all $s^* \in [-1,1]$,

$$\overline{\delta}_n(u;t) = \frac{1}{2}\left\{\partial_{2n-1}\left[k(t,s)\,u(s)\right]\right\}_{s=-1}^{s=1} + \varepsilon_n^*, \tag{56}$$

from which we require $u(s)$ to be $(2n-1)$-times continuously differentiable with respect to s because, by construction (see Eq. 4), $k(t,s)$ is infinitely so. Ignoring second-order terms of order $O(\beta_n \varepsilon_n^*)$, we define a mean predicted error by

$$(\overline{\mathscr{E}}_n u)(t) = \beta_n \overline{\delta}_n(u;t), \tag{57}$$

and also the further error discrepancies

$$\Delta \mathscr{E}_n^* u \equiv (\mathscr{E}_n - \mathscr{E}_n^*)u \quad \text{and} \quad \Delta \overline{\mathscr{E}}_n u \equiv (\mathscr{E}_n - \overline{\mathscr{E}}_n)u. \tag{58}$$

4 Test problems, results and discussion

With a prespecified solution $u(s)$, kernel factor $k(t,s)$ and parameters μ and ν, both the source function $f(t)$ of Eq. 4 and the quadrature rule $\mathscr{K}_n$ of Eq. 15 can be generated in order to test the theory of §2, because the error discrepancies in Eq. 58 may be computed explicitly using Eq. 51 and Eq. 57. The theory is tested on an example with kernel $K(T,S) = e^{-T^2 S}$ and known solution $U(S) = e^S \cos S$, using $n = 2,4,6,8$ in Eq. 58, with parameters $a = -\frac{3}{5}$, $b = \frac{2}{3}$, $\mu = \frac{1}{2}$ and $\nu = \frac{1}{3}$. In this and all subsequent examples, the source function $F(T)$ of Eq. 2 was obtained exactly using an algebraic manipulator, but its explicit form is omitted because it is both cumbersome and unenlightening.

Results of this test problem are presented in figure 1. First, in this (Gauss-Jacobi-quadrature) example, note that $\Delta \overline{\mathscr{E}}_n$ is, by design, uniformly considerably smaller than $\Delta \mathscr{E}_n^*$; the same qualitative behaviour is evident for numerous other examples. On this basis, and because of its unambiguous computability, we use $\overline{\mathscr{E}}_n u(t)$ as the error estimate $\widetilde{\mathscr{E}}_n u(t)$ in the modified Nyström method proposed in Eq. 43. Second, figure 1 corroborates the required global norm convergence to zero (see Eq. 24) of $\Delta \overline{\mathscr{E}}_n$ with increasing n. Third, the deviation of $\Delta \overline{\mathscr{E}}_n$ from the plane $\Delta \mathscr{E}_n = 0$ quantifies the magnitude of the second-order terms, of order $O(\beta_n \varepsilon_n^*)$, neglected in the approximation of Eq. 57. Figure 2 shows this deviation as a discrepancy between the actual computed error $\mathscr{E}_n u(t)$ and the mean-value predicted error $\overline{\mathscr{E}}_n u(t)$ for the test problem of figure 1. It is clear that this deviation imposes a restriction on the number M of recursions that can meaningfully be incorporated in Eq. 43.

With $\widetilde{\mathscr{E}}_n$ approximated by the specific functional form of $\overline{\mathscr{E}}_n$ in Eq. 57, the deferred discussion of the components $(\widetilde{\mathscr{E}}_n^{(\lambda,M)} \boldsymbol{K})_{ij}$ and $(\widetilde{\mathscr{E}}_n^{(\lambda,M)} \boldsymbol{f})_i$ of the matrices in Eq. 46 can be resumed. Defining the notation

$$\mathscr{D}_{n,r}[F(s_r)] \equiv \frac{\lambda \, \beta_n}{2} \frac{\partial^{2n-1}}{\partial s_r^{2n-1}} [F(s_r)] \Big|_{s_r=-1}^{s_r=1}, \tag{59}$$

we may deduce by direct computation, using Eq. 15 and Eq. 40, that

$$
\begin{aligned}
(\widetilde{\mathscr{E}}_n^{(\lambda,M)} \boldsymbol{K})_{ij} &= c_{j,n} \big(\mathscr{D}_{n,1}[k(\sigma_i,s_1) k(s_1,\sigma_j)] \\
&+ \mathscr{D}_{n,1} \big[k(\sigma_i,s_1) \mathscr{D}_{n,2}[k(s_1,s_2) k(s_2,\sigma_j)] \big] + \dots \big)
\end{aligned}
\tag{60}
$$

and

$$(\widetilde{\mathscr{E}}_n^{(\lambda,M)} \boldsymbol{f})_i = \mathscr{D}_{n,1}[k(\sigma_i,s_1) f(s_1)] + \mathscr{D}_{n,1} \big[k(\sigma_i,s_1) \mathscr{D}_{n,2}[k(s_1,s_2) f(s_2)] \big] + \dots, \tag{61}$$

in which the sums terminate with the term in $\mathscr{D}_{n,M}$. Although the right-hand sides of Eq. 60 and Eq. 61 can be re-expressed more efficiently in terms of nested operation,

we refrain from doing so because, by Eq. 59, they are series in increasing powers of β_n in which, by Eq. 54, each term is an exponentially small perturbation of the sum of all previous terms. Because of both this and the aforementioned limitations imposed by the omission of terms of order $O(\beta_n \varepsilon_n^*)$, only the first few terms in the sum in Eq. 40 will therefore need to be computed in practice, a maximum of $M = 3$ sufficing in the numerical experiments below.

The new method defined by Eq. 46, Eq. 60 and Eq. 61 has been implemented and validated on a number of test problems with known solutions. For the results in
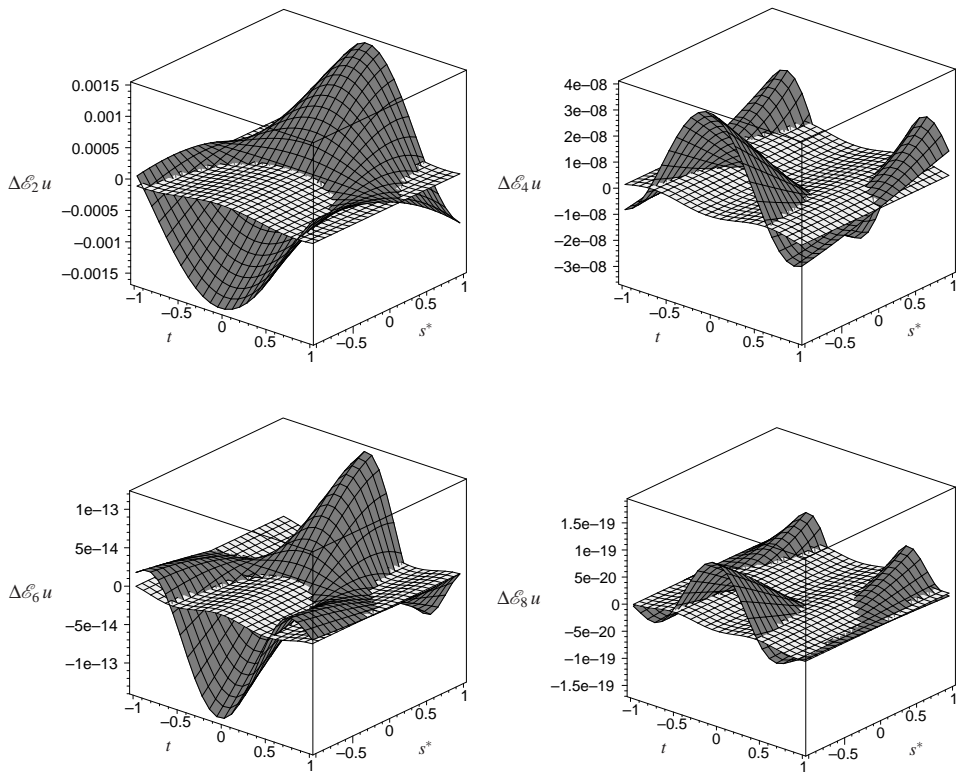
Figure 1: *Error discrepancies $\Delta\mathscr{E}_n^* u(t, s^*)$ (dark) and $\Delta\overline{\mathscr{E}}_n u(t)$ (light) for $n = 2, 4, 6, 8$ in Eq. 58, computed using $a = -\frac{3}{5}$, $b = \frac{2}{3}$, $\mu = \frac{1}{2}$, $\nu = \frac{1}{3}$ and $K(T, S) = e^{-T^2 S}$ with the test solution $U(S) = e^S \cos S$ in the integral in Eq. 2 (so that $k(t, s)$ and $u(s)$ are obtained from Eq. 3). The estimate $\Delta\overline{\mathscr{E}}_n u(t)$ is both smaller in modulus and more uniform than the standard error term $\Delta\mathscr{E}_n^* u(t, s^*)$; the (light) plane $\Delta\mathscr{E}_n^\mathscr{O} \equiv 0$ would indicate Eq. 57 to be the exact global error estimate for the Gauss-Jacobi quadrature of Eq. 15.*
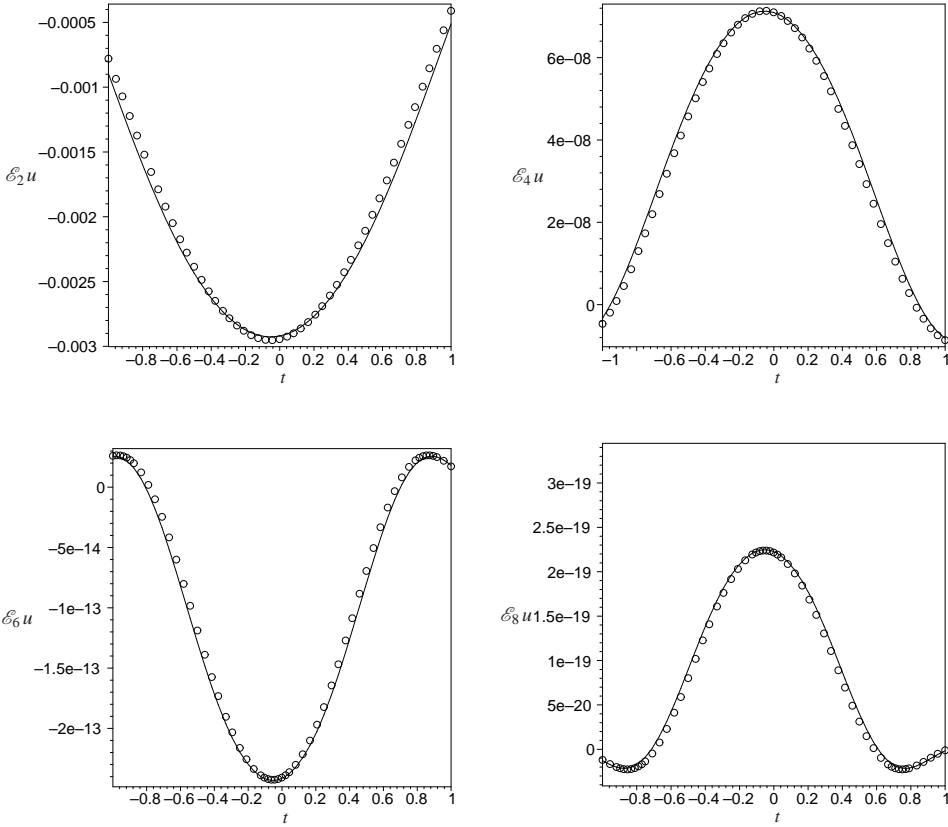
Figure 2: *Actual error $\mathcal{E}_n u(t)$ (solid line) and predicted error $\overline{\mathcal{E}}_n u(t)$ (circles) for $n = 2, 4, 6, 8$ in Eq. 58, computed using the Gauss-Jacobi quadrature of Eq. 15 for the example defined in the caption of figure 1. The discrepancy between the curves clearly scales with β_n, and reflects the omission of second- and higher-order terms in Eq. 57.*

figure 3, we use the parameters $\mu = \nu = 0$, and find that all results obtained are identical (to machine precision) to those generated independently using standard (tabulated) Gauss-Legendre quadrature. Figure 3 shows the *modified Nyström error* on $[-1, 1]$, defined by

$$e_n^{(\lambda, M)} u(t) \equiv ||u - \overline{u}_n^{(M)}||_\infty, \qquad M \geq 0, \tag{62}$$

for the lowest possible order of quadrature, $n = 2$ (in keeping with our aim); each separate sub-figure is for a fixed value of λ, and separate curves on each sub-figure are for different values of M. The method is computationally efficient: on a desktop

PC with a 1.6GHz CPU, the times required to obtain solutions for $M = 0$, 1, 2 and 3 were respectively 0.015, 0.109, 0.437 and 1.248 seconds.
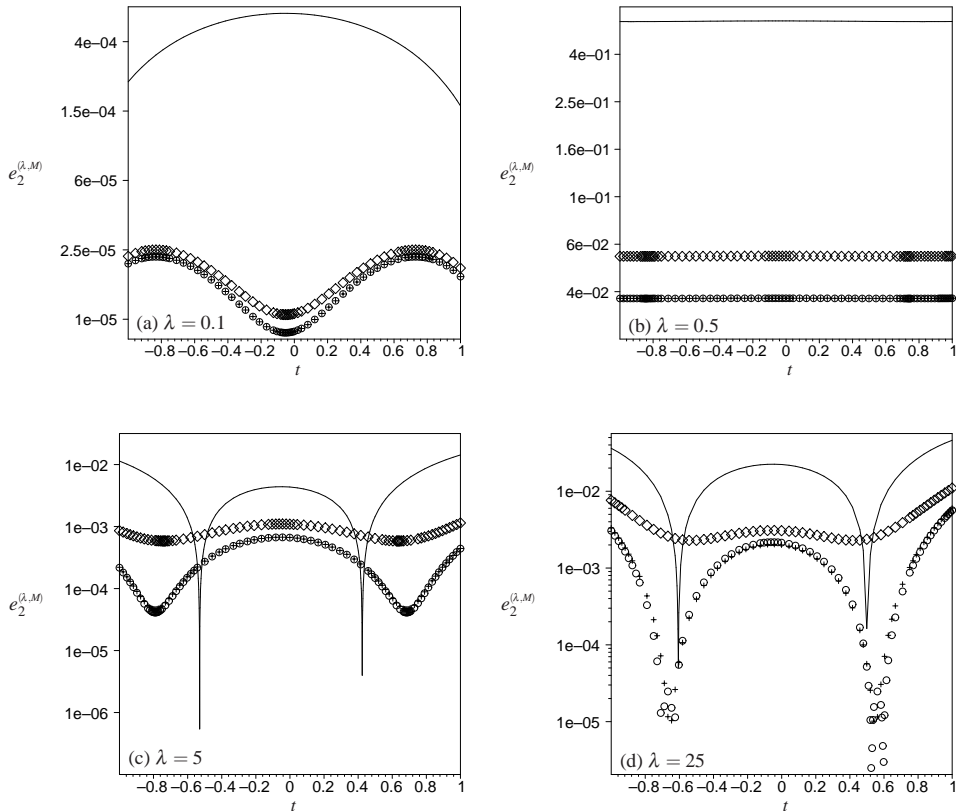

Figure 3: *Modified Nyström errors $e_n^{(\lambda,M)} u(t)$ of Eq. 62 for fixed $n = 2$ and different values of λ computed using the Gauss-Jacobi quadrature of Eq. 15 for the test problem described in the caption of figure 1, but with the new parameters $\mu = \nu = 0$. Successive modifications of the standard Nyström error, $M = 0$, (——) are shown by $M = 1$ (◇), $M = 2$ (○) and $M = 3$ (+). Validating computations using standard Gauss-Legendre quadrature yield results indistinguishable from those presented.*

By Eq. 59, the mth correction to the standard Nyström error is of order $O(\lambda^m \beta_n^m)$, hence corrections converge rapidly to zero with m when $|\lambda| \ll 1$. Although this explains the negligible effect of the $M = 3$ correction in figure 3(a), we note the impressive error reduction due to the first correction, i.e. $M = 1$; we recall that this is from *only two quadrature nodes*, i.e. a potential hand calculation. As $|\lambda|$ is increased to order $O(1)$ as in figure 3(b), the aforementioned convergence is
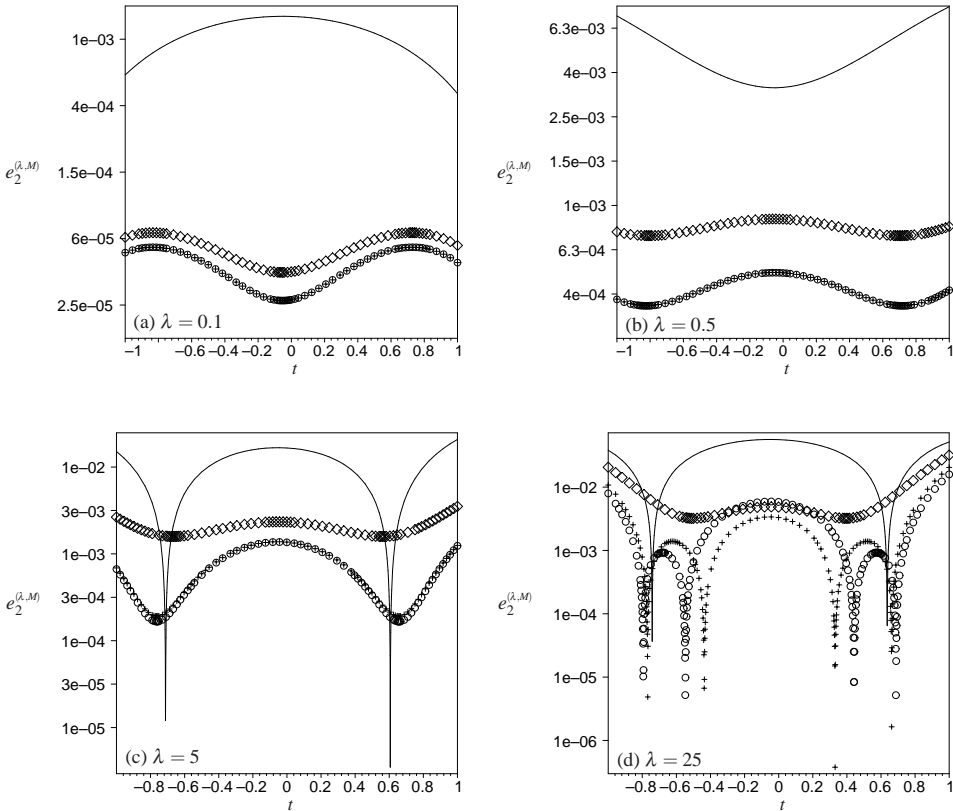
Figure 4: *Modified Nyström errors $e_n^{(\lambda,M)} u(t)$ of Eq. 62 for fixed $n = 2$ and different values of λ computed using the Gauss-Jacobi quadrature of Eq. 15 for the test problem described in the caption of figure 1, but with the new parameters $\mu = \nu = -\frac{1}{2}$. Successive modifications of the standard Nyström error, $M = 0$, (——) are shown by $M = 1$ ($\diamond$), $M = 2$ ($\circ$) and $M = 3$ (+). Validating computations using standard Gauss-(first-kind-)Chebyshev quadrature yield results indistinguishable from those presented.*

tempered; again, the $M = 2$ and $M = 3$ corrections are indistinguishable. As $|\lambda|$ is increased further to $|\lambda| \gg 1$, the truncation condition in Eq. 42 becomes more difficult to satisfy, upon which the solutions of the truncated Eq. 43 and the full Eq. 41 are expected to diverge.

Such divergence is apparent in figures 3(c) and 3(d); although $|\lambda| \gg 1$ in the latter of these, the performance of the modified method in 3(d) is comparable to that in 3(c) because the larger value of λ in Eq. 11 has similarly adversely affected the
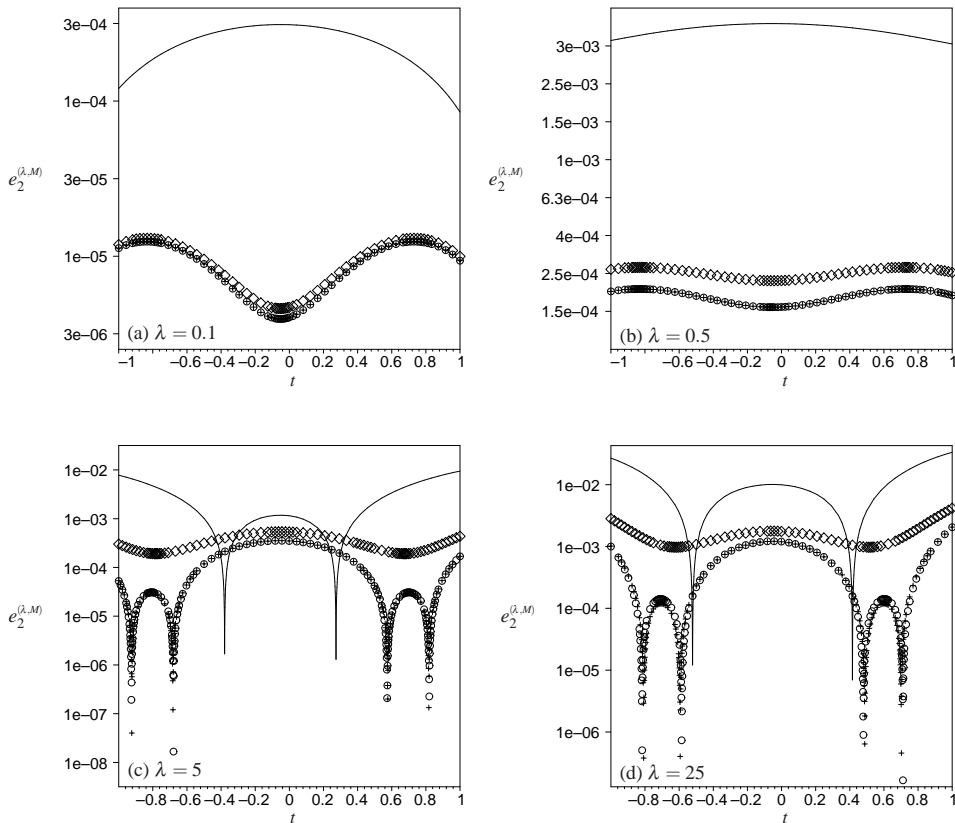
Figure 5: *Modified Nyström errors $e_n^{(\lambda,M)} u(t)$ of Eq. 62 for fixed $n = 2$ and different values of λ computed using the Gauss-Jacobi quadrature of Eq. 15 for the test problem described in the caption of figure 1, but with the new parameters $\mu = \nu = \frac{1}{2}$. Successive modifications of the standard Nyström error, $M = 0$, (——) are shown by $M = 1$ ($\diamond$), $M = 2$ ($\circ$) and $M = 3$ ($+$). Validating computations using Gauss-(second-kind-)Chebyshev quadrature yield results indistinguishable from those presented.*

performance of the standard method ($M = 0$). Note also from figures 3(c) and 3(d) that the $M = 2$ and $M = 3$ corrections are somewhat less uniform on $[-1, 1]$ than the $M = 1$ correction; again, this is a manifestation of the approach to the violation of the condition in Eq. 42. The trends seen in figure 3 reoccur in figures 4 and 5, in which $\mu = \nu = -\frac{1}{2}$ and $\mu = \nu = \frac{1}{2}$ respectively; in these cases, all results obtained are identical (to machine precision) to those generated independently using Gauss-Chebyshev quadrature of, respectively, the first and second kind.
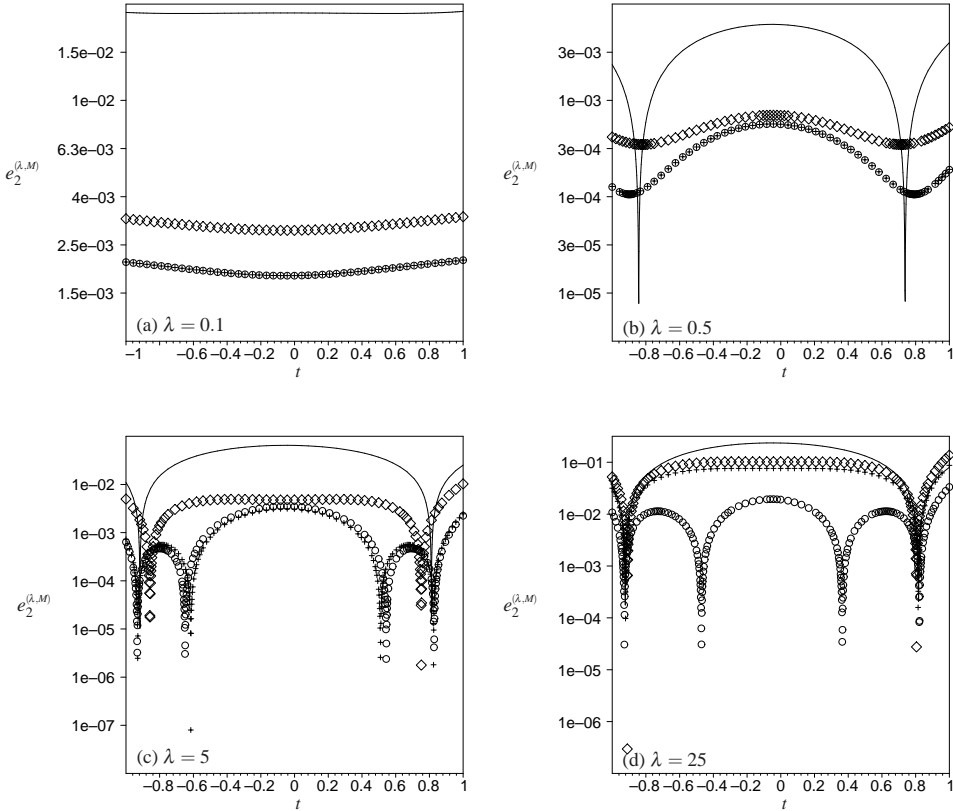
Figure 6: *Modified Nyström errors $e_n^{(\lambda,M)} u(t)$ of Eq. 62 for fixed $n = 2$ and different values of λ computed using the Gauss-Jacobi quadrature of Eq. 15 for the test problem described in the caption of figure 1, but with the new (singular) parameters $\mu = -\frac{4}{5}$ and $\nu = -\frac{9}{10}$. Successive modifications of the standard Nyström error, $M = 0$, (——) are shown by $M = 1$ (◇), $M = 2$ (○) and $M = 3$ (+).*

Figures 6 and 7 show results , for $n = 2$ and $n = 3$ respectively, for a challenging (more singular) example in which $\mu = -\frac{4}{5}$ and $\nu = -\frac{9}{10}$: the variation in n reveals two new features. First, figure 6(d) now demonstrates violation of the condition in Eq. 42, because for $|\lambda| \gg 1$ the errors for $M = 3$ are seen to be larger than those for $M = 2$; as figure 7(d) demonstrates, the condition in Eq. 42 can be recovered simply by increasing n from 2 to 3. Second, figure 7 reveals that there is no advantage to be gained by taking $M > 1$ when $n = 3$; the rapid convergence of β_n (see Eq. 54) means that the omitted error ε_n^* of Eq. 56 is the determining factor on the accuracy threshold that can be achieved. Further tests revealed that, when either μ or ν were
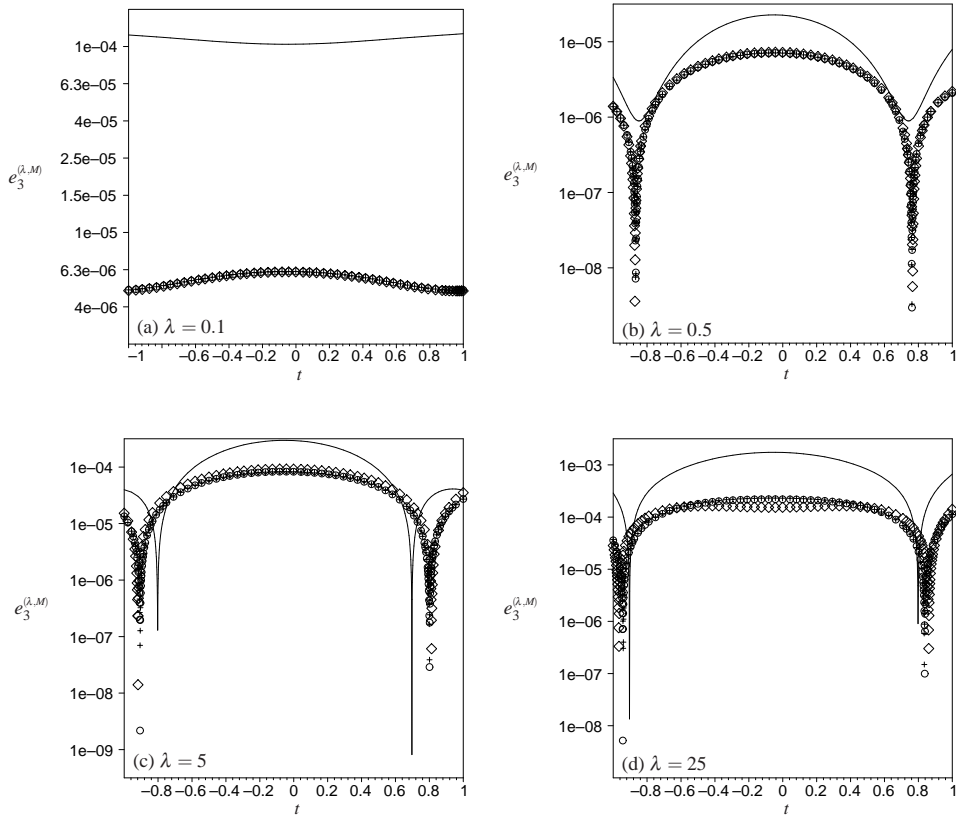
Figure 7: *Modified Nyström errors $e_n^{(\lambda,M)} u(t)$ of Eq. 62 for fixed $n = 3$ and different values of λ computed using the Gauss-Jacobi quadrature of Eq. 15 for the test problem described in the caption of figure 1, but with the new (singular) parameters $\mu = -\frac{4}{5}$ and $\nu = -\frac{9}{10}$. Successive modifications of the standard Nyström error, $M = 0$, (——) are shown by $M = 1$ (⋄), $M = 2$ (○) and $M = 3$ (+).*

closer to the limiting value of -1 (the case $\nu = 0.999999$ was considered), results for $M > 1$ were indistinguishable from those for $M = 1$, irrespective of n.

We note that, since $\lambda = \Lambda[(b-a)/2]^{\mu+\nu+1}$, increasing the length of the interval $[a,b]$ in the original FIE2 of Eq. 2 also acts to violate the condition in Eq. 42 for which the new method works. However, this is simply consistent with the corresponding degradation of the standard Nyström method for which, under such circumstances, composite rules (Ralston and Rabinowitz (2001), §4.9) can be used to recover the required order of accuracy; we can similarly amend our technique accordingly. Refinement of the present method requires improved estimates of $\mathcal{E}_n u(t)$

in order to shed light on the nature of the second- and higher-order terms neglected in Eq. 57; in particular, of a functional form of the error term ε_n^*. Further investigations are motivated on combining the new approach with product Nyström methods for kernels that are singular and/or non-infinitely differentiable, but not of a form described by Eq. 2. Finally, extension of the ideas in this paper to integral equations for higher-dimensional singular boundary value problems (e.g. Liu (2007a) and Liu (2007b)) should present no conceptual difficulty, although it is anticipated that the algebraic complexity in deriving the matrix and vector entries in Eq. 60 and Eq. 61 would increase considerably.

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