

NOTES ON TWO DEFINITE QUADRATURE FORMULAE OF ORDER THREE

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In two recent papers from 2017 and 2018 two definite quadrature formulae of order three were obtained which are modifications of the compound trapezium and midpoint quadrature rules, respectively. The criteria applied to the construction of these definite quadrature formulae is minimization of their error constants through the usage of appropriate formulae for numerical differentiation. In this note, we show that the aforementioned definite quadrature formulae also meet another criteria for optimality. For integrands having a continuous third derivative with a permanent sign, we present another error estimates, which are easier to evaluate and in many cases provide better error bounds.

Keywords: definite quadrature formulae, Peano kernel representation, Euler-Maclaurin summation formulae, a posteriori error estimates

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1. INTRODUCTION AND STATEMENT OF THE RESULTS

The definite integral

$$I[f] := \int_0^1 f(x) dx \quad (1.1)$$

is usually approximated by quadrature formulae, which are linear functionals of the form

$$Q[f] = \sum_{i=1}^n a_i f(x_i), \quad 0 \leq x_1 < \cdots < x_n \leq 1. \quad (1.2)$$

Throughout this paper, π_m stands for the set of real-valued algebraic polynomials of degree at most m . A quadrature formula Q has algebraic degree of precision

m (in short, $\text{ADP}(Q) = m$) if m is the largest non-negative integer such that its remainder functional

$$R[Q; f] := I[f] - Q[f]$$

vanishes whenever $f \in \pi_m$, and $R[Q; f] \neq 0$ when f is a polynomial of degree $m+1$. Let us recall that quadrature formula (1.2) is *definite of order* $r \in \mathbb{N}$, if there exists a real non-zero constant $c_r(Q)$ such that its remainder functional admits the representation

$$R[Q; f] = I[f] - Q[f] = c_r(Q)f^{(r)}(\xi)$$

for every real-valued function $f \in C^r[0, 1]$ with some $\xi \in [0, 1]$ depending on f . Furthermore, Q is called *positive definite* (resp., *negative definite*) of order r , if $c_r(Q) > 0$ ($c_r(Q) < 0$).

Definite quadrature formulae of order r provide one-sided approximation to $I[f]$ whenever $f^{(r)}$ has a permanent sign in the integration interval. For the sake of brevity, we introduce the following definition.

Definition 1.1. A real-valued function $f \in C^r[0, 1]$ is called r -positive (resp., r -negative) if $f^{(r)}(x) \geq 0$ (resp. $f^{(r)}(x) \leq 0$) for every $x \in [0, 1]$.

If $\{Q^+, Q^-\}$ is a pair of positive and negative definite quadrature formulae of order r , then $Q^+[f] \leq I[f] \leq Q^-[f]$ for every r -positive function f . This simple observation serves as a base for the derivation of a posteriori error estimates and rules for termination of calculations (stopping rules) in the algorithms for automatic numerical integration (see [3] for a survey). Most quadratures used in practice (e.g., quadrature formulae of Gauss, Radau, Lobatto, Newton-Cotes) are definite of certain order. The compound midpoint and trapezium rules

$$Q_n^{\text{Mi}}[f] = \frac{1}{n} \sum_{k=1}^n f\left(\frac{2k-1}{2n}\right), \quad Q_{n+1}^{\text{Tr}}[f] = \frac{1}{2n} (f(0) + f(1)) + \frac{1}{n} \sum_{k=1}^{n-1} f\left(\frac{k}{n}\right) \quad (1.3)$$

are the best known definite quadratures, they are respectively positive and negative definite of order two with error constants $c_2(Q_n^{\text{Mi}}) = \frac{1}{24n^2}$ and $c_2(Q_{n+1}^{\text{Tr}}) = -\frac{1}{12n^2}$. Definite quadrature formulae of order three, which are appropriately modified compound trapezium and midpoint quadratures, were constructed in [1] and [2]. The optimal definite quadrature formulae of higher order are not known explicitly, although their existence and uniqueness is known, see [5–7]. Asymptotically optimal definite quadrature formulae of fourth order were constructed in [3].

Theorem A ([1, part of Theorem 1]). *For every $n \geq 8$, the quadrature formula*

$$Q_n[f] = \sum_{k=0}^{n-1} A_{k,n} f(x_{k,n}), \quad x_{k,n} = \frac{k}{n}$$

with coefficients $A_{k,n} = 1/n$, $3 \leq k \leq n-4$, and

$$\begin{aligned} A_{0,n} &= \frac{81 + \sqrt{3}}{216n}, & A_{1,n} &= \frac{126 - \sqrt{3}}{108n}, & A_{2,n} &= \frac{207 + \sqrt{3}}{216n}, \\ A_{n-3,n} &= \frac{297 - \sqrt{3}}{216n}, & A_{n-2,n} &= \frac{\sqrt{3} - 18}{108n}, & A_{n-1,n} &= \frac{495 - \sqrt{3}}{216n}, \end{aligned}$$

is positive definite of order three with the error constant

$$c_3(Q_n) = \frac{\sqrt{3}}{216n^3} + \frac{27 - \sqrt{3}}{72n^4}. \quad (1.4)$$

Theorem B ([2, part of Theorem 1]). For every $n \in \mathbb{N}$, $n \geq 8$, the quadrature formula

$$Q_n^*[f] = \sum_{k=0}^{n+1} A_{k,n} f(y_{k,n})$$

with nodes $y_{0,n} = 0$, $y_{k,n} = \frac{2k-1}{2n}$, $k = 1, \dots, n$, $y_{n+1,n} = 1$ and coefficients

$$\begin{aligned} A_{0,n} &= \frac{-42+41\sqrt{3}}{162n}, & A_{1,n} &= \frac{678-203\sqrt{3}}{432n}, \\ A_{2,n} &= \frac{357+199\sqrt{3}}{648n}, & A_{3,n} &= \frac{164-13\sqrt{3}}{144n}, \\ A_{n-2,n} &= \frac{225-\sqrt{3}}{216n}, & A_{n-1,n} &= \frac{189+2\sqrt{3}}{216n}, \\ A_{n,n} &= \frac{234-\sqrt{3}}{216n}, & A_{n+1,n} &= 0, \end{aligned}$$

$A_{k,n} = 1/n$, $4 \leq k \leq n-3$, is positive definite of order three with the error constant

$$c_3(Q_n^*) = \frac{\sqrt{3}}{216n^3} + \frac{169\sqrt{3} - 210}{2592n^4}. \quad (1.5)$$

We need one more definition.

Definition 1.2 ([2]). The quadrature formula Q in (1.2) is called symmetrical, if $a_k = a_{n+1-k}$ and $x_k = 1 - x_{n+1-k}$ for $k = 1, \dots, n$, and nodes-symmetrical, if only the requirement for the nodes is satisfied.

The quadrature formula $\tilde{Q}[f] = \tilde{Q}[Q; f] := \sum_{k=1}^n a_k f(x_{n+1-k})$ is called a reflected quadrature formula for (1.2).

Some advantages of the definite quadrature formulae in Theorems A and B become clear when taking into account the following proposition.

Proposition 1.3 ([2]).

- (i) If Q is a positive definite quadrature formula of order r (r is odd), then its reflected quadrature formula \tilde{Q} is negative definite of order r and vice versa. Moreover, $c_r(\tilde{Q}) = -c_r(Q)$.
- (ii) If quadrature formula Q in (i) is nodes-symmetrical and definite of order r (r is odd), and f is an r -positive function, then with Q^* standing for either Q or \tilde{Q} we have

$$|R[Q^*; f]| \leq B[Q; f] := \left| \sum_{k=1}^{[n/2]} (a_k - a_{n+1-k})(f(x_{n+1-k}) - f(x_k)) \right|.$$

- (iii) Under the same assumptions for Q and f as in (ii), for $\hat{Q} = (Q + \tilde{Q})/2$ we have

$$|R[\hat{Q}; f]| \leq \frac{1}{2} B[Q; f].$$

In view of Proposition 1.3(i), the reflected quadratures to the quadrature formulae of Theorems A and B are negative definite of order three. Since they (and their reflected) are nodes-symmetrical and use equispaced nodes, one can apply Proposition 1.3(ii), (iii) to derive simple error bounds in terms of only a few integrand's values provided the integrand is three-positive or three-negative function. Of course, at our disposal are also the error estimates

$$|R[Q_n; f]| \leq c_3(Q_n) \|f'''\|_{C[0,1]} \quad (1.6)$$

with the error constants given in (1.4) or (1.5). However, this requires knowledge of $\|f'''\|_{C[0,1]}$, which may be unavailable or difficult to obtain. Here we propose alternative error estimates for the definite quadrature formulae in Theorems A and B, which require only knowledge of the values of the integrand's second derivative at the end-points.

Theorem 1.4. *Let Q_n be the quadrature formula in Theorem A. If f is three-positive or three-negative function, then*

$$|R[Q_n; f]| \leq \frac{0.277223}{n^3} |f''(1) - f''(0)|. \quad (1.7)$$

Theorem 1.5. *Let Q_n be the quadrature formula in Theorem B. If f is three-positive or three-negative function, then*

$$|R[Q_n; f]| \leq \frac{0.0369563}{n^3} |f''(1) - f''(0)|. \quad (1.8)$$

The rest of the paper is structured as follows. In Section 2 we provide a brief introduction to Peano's integral representation of linear functionals which vanish on π_{r-1} . The proofs of Theorem 1.4 and Theorem 1.5 are given in Section 3 and Section 4, respectively.

2. PEANO KERNEL REPRESENTATION OF LINEAR FUNCTIONALS

By $W_1^r[0, 1]$, $r \in \mathbb{N}$, we denote the Sobolev class of functions

$$W_1^r[0, 1] := \left\{ f \in C^{r-1}[0, 1]: f^{(r-1)} \text{ abs. continuous, } \int_0^1 |f^{(r)}(t)| dt < \infty \right\}.$$

In particular, $W_1^r[0, 1]$ contains the class $C^r[0, 1]$. If \mathcal{L} is a linear functional defined in $W_1^r[0, 1]$ that vanishes on π_{r-1} , then, by a classical result of Peano [9], \mathcal{L} admits the integral representation

$$\mathcal{L}[f] = \int_0^1 K_r(t) f^{(r)}(t) dt, \quad K_r(t) = \mathcal{L} \left[\frac{(\cdot - t)_+^{r-1}}{(r-1)!} \right], \quad t \in [0, 1],$$

where $u_+(t) = \max\{t, 0\}$, $t \in \mathbb{R}$.

In the case when \mathcal{L} is the remainder $R[Q; \cdot]$ of a quadrature formula Q with $\text{ADP}(Q) \geq r - 1$, the function $K_r(t) = K_r(Q; t)$ is referred to as the r -th Peano kernel of Q . For Q as in (1.2), explicit representations for $K_r(Q; t)$, $t \in [0, 1]$, are

$$K_r(Q; t) = \frac{(1-t)^r}{r!} - \frac{1}{(r-1)!} \sum_{i=1}^n a_i (x_i - t)_+^{r-1}, \quad (2.1)$$

$$K_r(Q; t) = (-1)^r \left[\frac{t^r}{r!} - \frac{1}{(r-1)!} \sum_{i=1}^n a_i (t - x_i)_+^{r-1} \right]. \quad (2.2)$$

Since for $f \in C^r[0, 1]$ we have

$$R[Q; f] = \int_0^1 K_r(Q; t) f^{(r)}(t) dt, \quad (2.3)$$

it is clear that Q is a positive (negative) definite quadrature formula of order r if and only if $\text{ADP}(Q) = r - 1$ and $K_r(Q; t) \geq 0$ (resp. $K_r(Q; t) \leq 0$) for all $t \in [0, 1]$. The following lemma is an immediate consequence of this observation.

Lemma 2.1. *Assume that Q is a positive or negative definite quadrature formula of order r . If f is an r -positive or r -negative function, then*

$$|R[Q; f]| \leq \max_{t \in [0, 1]} |K_r(Q; t)| \cdot \left| f^{(r-1)}(1) - f^{(r-1)}(0) \right|. \quad (2.4)$$

The proofs of Theorems 1.4 and 1.5 make use of this lemma.

3. PROOF OF THEOREM 1.4

We start with recalling the way the quadrature formula in Theorem A was obtained. Assuming $f \in W_1^3[0, 1]$, then a particular case of the Euler-Maclaurin summation formula (c.f. [4, Satz 98]) yields

$$I[f] = Q_{n+1}^{\text{Tr}}[f] - \frac{1}{12n^2} [f'(1) - f'(0)] - \frac{1}{n^3} \int_0^1 B_3(nx - \{nx\}) f'''(x) dx. \quad (3.1)$$

Here $\{\cdot\}$ is the fractional part function and B_3 is the third Bernoulli polynomial with leading coefficient $1/6$,

$$B_3(x) = \frac{x^3}{6} - \frac{x^2}{4} + \frac{x}{12}.$$

Writing (3.1) in the equivalent form

$$\begin{aligned} I[f] &= Q_{n+1}^{\text{Tr}}[f] - \frac{1}{12n^2} [f'(1) - f'(0)] - \frac{\sqrt{3}}{216n^3} [f''(1) - f''(0)] \\ &\quad + \frac{1}{n^3} \int_0^1 \left(\frac{\sqrt{3}}{216} - B_3(nx - \{nx\}) \right) f^{(3)}(x) dx \\ &=: \tilde{Q}[f] + R[\tilde{Q}; f], \end{aligned} \quad (3.2)$$

we observe that the quadrature formula \tilde{Q} in the first line of (3.2) is positive definite of order three though not of the desired form as it involves values of the first and the second derivatives of the integrand. Therefore, the expressions with derivatives $f^{(j)}(0)$ resp. $f^{(j)}(1)$, $j = 1, 2$, are replaced by one-parametric linear combinations of $\{f(x_{i,n})\}_{i=0}^3$ resp. $\{f(x_{n-i,n})\}_{i=0}^3$ (i.e., numerical differentiation formulae) which evaluate these expressions to the exact value whenever $f \in \pi_2$. The resulting quadrature formula Q has nodes $x_{k,n} = k/n$, $k = 0, \dots, n$, and weights $A_{k,n} = 1/n$, $4 \leq k \leq n-4$, while $\{A_{k,n}\}_0^3$ depend on a single parameter, say θ , and $\{A_{k,n}\}_{n-3}^n$ depend on another single parameter, say ϱ . Specifically, we have

$$\begin{aligned} A_{0,n} &= \frac{108 - \theta}{216n}, & A_{1,n} &= \frac{171 + \sqrt{3} + 3\theta}{216n}, \\ A_{2,n} &= \frac{288 - 2\sqrt{3} - 3\theta}{216n}, & A_{3,n} &= \frac{189 + \sqrt{3} + \theta}{216n}, \\ A_{n-3,n} &= \frac{189 - \sqrt{3} + \varrho}{216n}, & A_{n-2,n} &= \frac{288 + 2\sqrt{3} - 3\varrho}{216n}, \\ A_{n-1,n} &= \frac{171 - \sqrt{3} + 3\varrho}{216n}, & A_{n,n} &= \frac{108 - \varrho}{216n}. \end{aligned}$$

On the interval $[x_{3,n}, x_{n-3,n}]$ the third Peano kernel of Q coincides with that of \tilde{Q} in (3.2), i.e.,

$$K_3(Q; t) = \frac{1}{n^3} \left(\frac{\sqrt{3}}{216} - B_3(nt - \{nt\}) \right) \geq 0, \quad t \in [x_{3,n}, x_{n-3,n}]. \quad (3.3)$$

It has been shown in [1, Section 3] that the requirement $K_3(Q; t) \geq 0$ on $(0, x_{3,n})$ and on $(x_{n-3,n}, 1)$ is equivalent respectively to $\theta \leq \theta^* = 27 - \sqrt{3}$ and $\varrho \geq \varrho^* = 108$. In the limit case $(\theta, \varrho) = (\theta^*, \varrho^*)$, Q becomes the quadrature formula Q_n in Theorem 1.4 (note that $A_{n,n} = 0$ in that case). According to [1, Eqns. (3.12) and (3.14)], the integrals

$$\int_0^{x_{3,n}} K_3(Q; t) dt \quad \text{and} \quad \int_{x_{n-3,n}}^1 K_3(Q; t) dt$$

are resp. monotonically decreasing and monotonically increasing functions of θ (resp. ϱ), therefore the choice $(\theta, \varrho) = (\theta^*, \varrho^*)$ is optimal in the sense that it provides the smallest error constant (1.4).

We are going to show that this choice is also optimal in another sense: it minimizes $\|K_3(Q; \cdot)\|_{C[0,1]}$ while preserving non-negativity of $K_3(Q; t)$ on $[0, 1]$. More precisely, we shall show that the choice $\theta = \theta^*$ minimizes $\max_{t \in [0, x_{3,n}]} K_3(Q; t)$ while the

choice $\varrho = \varrho^*$ minimizes $\max_{t \in [x_{n-3,n}, 1]} K_3(Q; t)$.

Using formula (2.2) for Peano kernels with $r = 3$, after the change of variable $t = u/n$ we arrive at the following representation of $K_3(Q; t)$ for $t \in [0, x_{3,n}]$

$$\begin{aligned} K_3(Q; t) &= -\frac{1}{6n^3} \left[u^3 - \frac{108-\theta}{72} u^2 - \frac{171+\sqrt{3}+3\theta}{72} (u-1)_+^2 - \frac{288-2\sqrt{3}-3\theta}{72} (u-2)_+^2 \right] \\ &=: -\frac{1}{6n^3} \varphi(\theta, u), \quad u \in [0, 3]. \end{aligned}$$

It is easily verified that

$$\frac{\partial \varphi}{\partial \theta} = -\frac{1}{72n^3} \left[u^2 - 3(u-1)_+^2 + 3(u-2)_+^2 \right] \leq 0, \quad u \in [0, 3],$$

hence φ is a decreasing function of θ for every fixed $u \in [0, 3]$. Consequently,

$$\begin{aligned} \max_{t \in [0, x_{3,n}]} K_3(Q; t) &\geq \max_{u \in [0, 3]} \frac{-\varphi(\theta^*, u)}{6n^3} = \max_{t \in [0, x_{3,n}]} K_3(Q_n; t) \\ &= \frac{1}{432n^3} \max_{u \in [0, 3]} \left[-72u^3 + (81 + \sqrt{3})u^2 + (252 - 2\sqrt{3})(u-1)_+^2 + (207 + \sqrt{3})(u-2)_+^2 \right]. \end{aligned}$$

By a straightforward calculation we find that the latter maximum is attained at $u_0 = (81 + \sqrt{3})/108 \in (0, 1)$ and

$$\max_{t \in [0, x_{3,n}]} K_3(Q_n; t) = \frac{1}{12n^3} \left(\frac{81 + \sqrt{3}}{108} \right)^3 < \frac{0.0375}{n^3}. \quad (3.4)$$

Now we estimate $\max_{t \in [x_{n-3,n}, 1]} K_3(Q; t)$. Using (2.1) with $r = 3$, we obtain

$$\begin{aligned} K_3(Q; t) &= \frac{(1-t)^3}{6} - \frac{1}{2} \sum_{k=0}^n A_{k,n} (x_{k,n} - t)_+^2 \\ &= \frac{(1-t)^3}{6} - \frac{1}{2} \sum_{k=0}^n A_{k,n} (1-t-x_{n-k,n})_+^2 \\ &\stackrel{x=1-t}{=} \frac{x^3}{6} - \frac{1}{2} \sum_{k=0}^n A_{n-k,n} (x-x_{k,n})_+^2 =: \tilde{K}_3(Q; x), \end{aligned}$$

where $x \in [0, x_{3,n}]$ when $t \in [x_{n-3,n}, 1]$. With the further change of variable $x = u/n$, $u \in [0, 3]$, we get

$$\begin{aligned} \tilde{K}_3(Q; x) &= \frac{1}{6n^3} \left[u^3 - \frac{108-\varrho}{72} u^2 - \frac{171-\sqrt{3}+3\varrho}{72} (u-1)_+^2 - \frac{288+2\sqrt{3}-3\varrho}{72} (u-2)_+^2 \right] \\ &=: \frac{1}{6n^3} \psi(\varrho, u). \end{aligned}$$

Since

$$\frac{\partial \psi}{\partial \varrho} = \frac{1}{72n^3} \left[u^2 - 3(u-1)_+^2 + 3(u-2)_+^2 \right] \geq 0, \quad u \in [0, 3],$$

we conclude that ψ is an increasing function of ϱ for every fixed $u \in [0, 3]$. Consequently,

$$\begin{aligned} \max_{t \in [x_{n-3,n}, 1]} K_3(Q; t) &= \max_{x \in [0, x_{3,n}]} \tilde{K}_3(Q; x) \\ &\geq \frac{1}{6n^3} \max_{u \in [0, 1]} \psi(\varrho^*, u) = \max_{t \in [x_{n-3,n}, 1]} K_3(Q_n; t) \\ &= \frac{1}{432n^3} \max_{u \in [0, 3]} \left[72u^3 - (495 - \sqrt{3})(u-1)_+^2 + (36 - 2\sqrt{3})(u-2)_+^2 \right] \\ &=: \frac{1}{432n^3} \max_{u \in [0, 3]} g(u). \end{aligned}$$

The maximum of $g(u)$ in $[0, 3]$ is attained at the point $u_1 = 1.4788175 \dots$, which is the smaller root of the quadratic equation

$$108u^2 - (495 - \sqrt{3})(u-1) = 0,$$

and

$$\max_{t \in [x_{n-3,n}, 1]} K_3(Q_n; t) = \frac{1}{432n^3} g(u_1) = \frac{0.2772229 \dots}{n^3} < \frac{0.277223}{n^3}. \quad (3.5)$$

Finally, from (3.3) we have

$$\max_{t \in [x_{3,n}, x_{n-3,n}]} K_3(Q_n; t) = \frac{2\|B_3\|_{C[0,1]}}{n^3} = \frac{\sqrt{3}}{108n^3} < \frac{0.0161}{n^3}. \quad (3.6)$$

From (3.4), (3.5) and (3.6) we conclude that

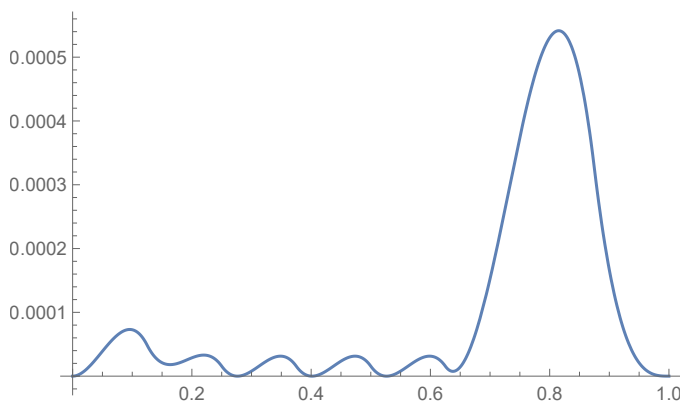
$$\max_{t \in [0, 1]} K_3(Q_n; t) < \frac{0.277223}{n^3}.$$

This inequality and Lemma 2.1 applied with $r = 3$ accomplish the proof of Theorem 1.4. Figure 1 depicts the Peano kernel $K_3(Q_8; t)$ and it shows that its greatest maximum in $[0, 1]$ is the rightmost one.

4. PROOF OF THEOREM 1.5

The starting point for derivation of the quadrature formula in Theorem B is the following identity, which is a consequence of another version of the Euler-Maclaurin summation formula (c.f. [4, Satz 98]):

$$\begin{aligned} I[f] &= Q_n^{\text{Mi}}[f] + \frac{1}{24n^2} [f'(1) - f'(0)] - \frac{\sqrt{3}}{216n^3} [f''(1) - f''(0)] \\ &\quad + \frac{1}{n^3} \int_0^1 \left(\frac{\sqrt{3}}{216} - B_3(\{nx + 1/2\}) \right) f^{(3)}(x) dx =: \overline{Q}[f] + R[\overline{Q}; f], \end{aligned}$$

Figure 1. Graph of $K_3(Q_8; t)$, Theorem 1.4

where

$$\overline{Q}[f] = Q_n^{\text{Mi}}[f] - \frac{1}{24n^2}f'(0) + \frac{\sqrt{3}}{216n^3}f''(0) + \frac{1}{24n^2}f'(1) - \frac{\sqrt{3}}{216n^3}f''(1). \quad (4.1)$$

Again, \overline{Q} is a positive definite quadrature formula, though not of the desired type as it involves values of integrand's derivatives, therefore the expressions with derivatives values at the end-points are replaced by pairs of formulae for numerical differentiation involving only integrand's values at the few closest nodes. This yields a quadrature formula Q with $\text{ADP}(Q) = 2$

$$Q[f] = \sum_{k=0}^{n+1} A_{k,n} f(y_{k,n}) \quad (4.2)$$

with nodes

$$y_{0,n} = 0, \quad y_{n+1,n} = 1, \quad y_{k,n} = \frac{2k-1}{2n}, \quad k = 1, \dots, n-1$$

and (for $n \geq 8$) weights $A_{k,n} = 1/n$, $4 \leq k \leq n-3$. The weights $\{A_{k,n}\}_{k=0}^3$ depend on a single parameter, say θ , while $\{A_{k,n}\}_{k=n-2}^{n+1}$ depend on another single parameter, say ϱ , these weights are given below

$$\begin{aligned} A_{0,n} &= \frac{\theta}{81n}, & A_{1,n} &= \frac{234 + \sqrt{3} - 5\theta}{216n}, \\ A_{2,n} &= \frac{567 - 6\sqrt{3} + 10\theta}{648n}, & A_{3,n} &= \frac{225 + \sqrt{3} - \theta}{216n}, \\ A_{n-2,n} &= \frac{225 - \sqrt{3} - \varrho}{216n}, & A_{n-1,n} &= \frac{567 + 6\sqrt{3} + 10\varrho}{648n}, \\ A_{n,n} &= \frac{234 - \sqrt{3} - 5\varrho}{216n}, & A_{n+1,n} &= \frac{\varrho}{81n}. \end{aligned}$$

On the interval $[y_{3,n}, y_{n-2,n}]$ the Peano kernel $K_3(Q; t)$ coincides with that of \overline{Q}

$$K_3(Q; t) = n^{-3} \left[\frac{\sqrt{3}}{216} - B_3(\{nt + 1/2\}) \right] \geq 0, \quad t \in [y_{3,n}, y_{n-2,n}], \quad (4.3)$$

thus care is to be taken only for finding the values of parameters θ and ϱ which ensure non-negativeness of $K_3(Q; t)$ on the intervals $[0, y_{3,n}]$ and $[y_{n-2,n}, 1]$. It has been shown in [2] that this is the case when $\theta \geq \theta^* = (41\sqrt{3} - 42)/2$ and $\varrho \leq \varrho^* = 0$. The quadrature formula Q_n in Theorem B is obtained from (4.2) with $(\theta, \varrho) = (\theta^*, \varrho^*)$ (and in this case $A_{n+1,n} = 0$). Since the integrals

$$\int_0^{y_{3,n}} K_3(Q; t) dt \quad \text{and} \quad \int_{y_{n-2,n}}^1 K_3(Q; t) dt$$

are respectively monotonically increasing function of θ and monotonically decreasing function of ϱ (see [2, equations (11) and (12)]), the choice $(\theta, \varrho) = (\theta^*, \varrho^*)$ is optimal in the sense that it provides the minimal error constant (1.5).

For the proof of Theorem 1.5 we need to find $\|K_3(Q_n; \cdot)\|_{C[0,1]}$, and this requires comparison of

$$\max_{t \in [0, y_{3,n}]} K_3(Q_n; t) \quad \text{and} \quad \max_{t \in [y_{n-2,n}, 1]} K_3(Q_n; t).$$

Similarly to the proof of Theorem 1.4, with a suitable change of the variable this task is reduced to comparison of the maxima of some spline functions independent of n on fixed intervals. Figure 2 depicts the Peano kernel $K_3(Q_8; t)$, showing that its greatest maximum in $[0, 1]$ is the rightmost one. This situation persists for every $n \geq 8$ (only the number of equi-oscillations of $K_3(Q_8; t)$ in $[y_{3,n}, y_{n-2,n}]$ changes). Therefore,

$$\|K_3(Q_n; \cdot)\|_{C[0,1]} = \max_{t \in [y_{n-2,n}, 1]} K_3(Q_n; t).$$

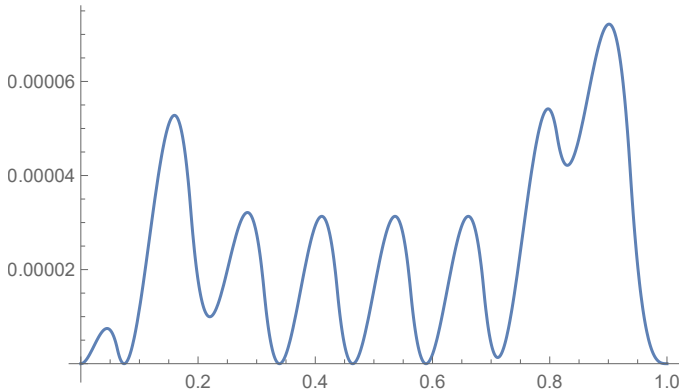


Figure 2. Graph of $K_3(Q_8; t)$, Theorem 1.5

From (2.2) with $r = 3$ we obtain

$$\begin{aligned} K_3(Q_n; t) &= \frac{(1-t)^3}{6} - \frac{1}{2} \sum_{k=0}^{n+1} A_{k,n} (y_{k,n} - t)_+^2 \\ &= \frac{(1-t)^3}{6} - \frac{1}{2} \sum_{k=0}^{n+1} A_{k,n} (1-t-y_{n+1-k,n})_+^2 \\ &\stackrel{x=1-t}{=} \frac{x^3}{6} - \frac{1}{2} \sum_{k=0}^{n+1} A_{n+1-k,n} (x-y_{k,n})_+^2 =: \tilde{K}_3(Q_n; x). \end{aligned}$$

We observe that $x \in [0, y_{3,n}]$ when t varies in $[y_{n-2,n}, 1]$. By substituting further $x = u/n$, $u \in [0, 5/2]$, we get

$$\tilde{K}_3(Q; x) = \frac{1}{432n^3} h(u), \quad u \in [0, 5/2],$$

where

$$h(u) = 72u^3 - (234 - \sqrt{3}) \left(u - \frac{1}{2}\right)_+^2 - (189 + 2\sqrt{3}) \left(u - \frac{3}{2}\right)_+^2.$$

The maximum of $h(u)$ in $[0, 5/2]$ is attained at the point $u_1 = 0.79073\dots$, which is the smaller root of the quadratic equation

$$216u^2 - (234 - \sqrt{3})(2u - 1) = 0,$$

and $h(u_1) < 15.9651065$, whence

$$\|K_3(Q_n; \cdot)\|_{C[0,1]} \leq \frac{1}{432n^3} h(u_1) < \frac{0.0369563}{n^3}.$$

Theorem 1.5 now follows from the above inequality and Lemma 2.1.

Remark 4.1. In [8] estimates similar to those in Theorems 1.4 and 1.5 are proved for the Radau-type quadrature formulae associated with the spaces of parabolic splines with double equidistant knots. These quadrature formulae are definite of order three, and under the assumptions of Theorems 1.4 and 1.5, the remainder $R[Q_{n+1}^R; f]$ of the $(n+1)$ -point Radau quadrature formula Q_{n+1}^R admits the much better error bound

$$|R[Q_{n+1}^R; f]| \leq \frac{\sqrt{3}}{108n^3} |f''(1) - f''(0)| < \frac{0.01604}{n^3} |f''(1) - f''(0)|.$$

However, since these quadrature formulae are not nodes-symmetrical, for them the error estimates implied by Proposition 1.3(ii),(iii) are not applicable.

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