ГОДИШНИК НА СОФИЙСКИЯ УНИВЕРСИТЕТ „СВ. КЛИМЕНТ ОХРИДСКИ“

ФАКУЛТЕТ ПО МАТЕМАТИКА И ИНФОРМАТИКА
Том 106

ANNUAL OF SOFIA UNIVERSITY „ST. KLIMENT OHRIDSKI“

FACULTY OF MATHEMATICS AND INFORMATICS
Volume 106

DEFINITE QUADRATURE FORMULAE OF 5-TH ORDER WITH EQUIDISTANT NODES

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We construct sequences of definite quadrature formulae of order five which use equidistant nodes. The error constants of these quadratures are evaluated and simple a posteriori error estimates derived under the assumption that the integrand's fifth derivative does not change its sign in the integration interval.

Keywords: Definite quadrature formulae, Peano kernels, Euler-MacLaurin summation formulae, a posteriori error estimates.
2000 Math. Subject Classification: 41A55, 65D30, 65D32.

1. INTRODUCTION AND STATEMENT OF THE RESULTS

The definite integral

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

is evaluated approximately by a quadrature formula, which is a linear functional of the form

$$Q[f] = \sum_{i=0}^{n} a_i\, f(x_i), \qquad 0 \le x_0 < x_1 < \cdots < x_n \le 1\,. \tag{1.1}$$

Two reasonable though rather demanding requirements for a quadrature formula (1.1) are : 1) to have the smallest possible maximal error for integrands f belonging to a given class of functions and 2) to provide the exact value of the integral for integrands from a linear space of the highest possible dimension. Quadrature formulae satisfying these two requirements are called *optimal* and *Gauss type* quadratures, respectively. Regardless which of these criteria is applied for the design of a quadrature formula, typically its nodes and weights are evaluated numerically, thus they are only approximately known. For this reason often in practice a preference is given to quadrature formulae having other useful properties, e.g. quadrature formulae whose knots and weights are *explicitly* known, or which allow easy error estimation. For instance, using quadrature formulae with equispaced nodes, we save half of the integrand evaluations when doubling the number of nodes; using quadrature formulae of (almost) Chebyshev type (i.e., with almost all weights equal to each other) we reduce the error induced by rounding. In automated routines for numerical integration, definite quadrature formulae are widely used for derivation of criteria for termination of calculations (the so-called stopping rules), see e.g. [5].

This paper is a continuation of our previous study on definite quadrature formulae of low order which use equidistant nodes and are of almost Chebyshev type. Before formulating our results, let us recall some definitions.

Quadrature formula (1.1) is said to have *algebraic degree of precision* m (in short, $ADP(Q) = m$), if its remainder

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

vanishes whenever $f \in \pi_m$, and $R[Q; f] \neq 0$ when f is a polynomial of degree $m+1$. Here and henceforth, π_k stands for the set of real algebraic polynomials of degree at most k.

Definition 1. Quadrature formula (1.1) is said to be *definite of order* r, $r \in \mathbb{N}$, 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 $c_r(Q) > 0$ ($c_r(Q) < 0$).

Definition 2. 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 $x \in [0, 1]$.

A definite quadrature formula of order r provides one-sided approximation to $I[f]$ whenever f is $r-$positive or $r-$negative. If $\{Q^+,\ Q^-\}$ is a pair of a positive and a negative definite quadrature formula of order r and f is an r-positive function, then $Q^+[f] \leq I[f] \leq Q^-[f]$. Most of quadrature formulae used in practice (e.g., quadrature formulae of Gauss, Radau, Lobatto, Newton-Cotes) are definite of certain order.

In [1] we constructed several sequences of asymptotically optimal definite quadrature formulae of order four with all but a few boundary nodes being equidistant. For some pairs of these definite quadrature formulae we derived a posteriori error estimates. In [2, 3] definite quadrature formulae of order three based on the nodes of compound trapesium and midpoint quadratures were constructed and a posteriori error estimates derived. It turns out that definite quadrature formulae of odd order offer some additional advantages, see Proposition 1 below.

Definition 3. Quadrature formula (1.1) is called:

- *symmetrical*, if

$$a_k = a_{n-k}\,, \qquad k = 0, \dots, n\,, \tag{1.2}$$
$$x_k = 1 - x_{n-k}\,, \qquad k = 0, \dots, n\,; \tag{1.3}$$

- *nodes-symmetrical*, if only condition (1.3) is satisfied;
- The quadrature formula

$$\widetilde{Q}[f] = \widetilde{Q}[Q; f] := \sum_{k=0}^{n} a_k\, f(x_{n-k}) \tag{1.4}$$

is called *reflected quadrature formula* to (1.1).

Proposition 1 ([**2**]). *(i) If Q is a positive definite quadrature formula of order r (r – odd), then its reflected quadrature formula $\widetilde{Q}$ is negative definite of order r and vice versa. Moreover, $c_r(\widetilde{Q}) = -c_r(Q)$.*

(ii) If quadrature formula Q in (1.1) is nodes-symmetrical and definite of order r (r – odd), and f is an r-positive or r-negative function, then, with Q^* standing for either Q or $\widetilde{Q}$ we have

$$\begin{aligned} \big|R[Q^*; f]\big| \le B[Q; f] &:= \big|\widetilde{Q}[f] - Q[f]\big| \\ &= \Big|\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \big(a_k - a_{n-k}\big)\big(f(x_{n-k}) - f(x_k)\big)\Big|. \end{aligned} \tag{1.5}$$

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

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

Proposition 1(i) implies that definite quadrature formulae of odd order are never symmetrical. Let us point out that the error estimate (1.5) becomes especially simple when almost all coefficients of Q are equal to each other.

For $n \in \mathbb{N}$ and a function f defined on the interval $[0,1]$, we denote

$$x_i = x_{i,n} = \frac{i}{n}\,, \quad f_i = f(x_{i,n})\,, \qquad i = 0\,\ldots, n\,.$$

Recall that the finite differences $\Delta^k f_i$ are defined recursively by

$$\Delta^1 f_i = \Delta f_i := f_{i+1} - f_i \quad \text{and} \quad \Delta^{k+1} f_i = \Delta\big(\Delta^k f_i\big)\,, \quad k \ge 1\,.$$

Set

$$c := \frac{3+\sqrt{30}}{21600}\sqrt{1 - 2\sqrt{\frac{2}{15}}}\,, \quad c \approx 0.000203818\,.$$

Our main result reads as follows:

Theorem 1. *(i) For every $n \ge 11$, the quadrature formula*

$$Q_n[f] = \frac{1}{n}\sum_{k=0}^{n-1} A_k\, f_k + \frac{c}{n}\big(\Delta^4 f_0 - \Delta^4 f_{n-5}\big)\,,$$

where $A_k = 1$ for $5 \le k \le n-6$ and

$$A_0 = \frac{95}{288}, \quad A_1 = \frac{317}{240}, \quad A_2 = \frac{23}{30}, \quad A_3 = \frac{793}{720}, \quad A_4 = \frac{157}{160},$$
$$A_{n-5} = \frac{383}{288}, \quad A_{n-4} = -\frac{481}{720}, \quad A_{n-3} = \frac{22}{5}, \quad A_{n-2} = -\frac{1823}{720}, \quad A_{n-1} = \frac{4277}{1440}\,,$$

is positive definite of order 5 with the error constant

$$c_5(Q_n) = \frac{c}{n^5} + \frac{5(19 - 288c)}{288 n^6}\,. \tag{1.6}$$

(ii) If f is a 5-positive or 5-negative function, then

$$\big|R[Q_n; f]\big| \le \frac{1}{n}\left|\Big(\frac{95}{288} - c\Big)\big(\Delta^5 f_0 + \Delta^5 f_{n-5}\big) + 2c\left(\Delta^4 f_{n-4} - \Delta^4 f_0\right)\right|.$$

As an immediate consequence of Theorem 1 and Proposition 1 we have:

Corollary 1. *The reflected to Q_n from Theorem 1 quadrature formula $\widetilde{Q}_n$ is negative definite of order 5 with the error constant $c_5(\widetilde{Q}_n) = -c_5(Q_n)$.*

If f is a 5-positive or 5-negative function and $\hat{Q}_n = \frac{1}{2}\big(Q_n + \widetilde{Q}_n\big)$, then

$$\big|R[\widetilde{Q}_n; f]\big| \le \frac{1}{n}\left|\Big(\frac{95}{288} - c\Big)\big(\Delta^5 f_0 + \Delta^5 f_{n-5}\big) + 2c\left(\Delta^4 f_{n-4} - \Delta^4 f_0\right)\right|.$$

$$\big|R[\hat{Q}_n; f]\big| \le \frac{1}{2n}\left|\Big(\frac{95}{288} - c\Big)\big(\Delta^5 f_0 + \Delta^5 f_{n-5}\big) + 2c\left(\Delta^4 f_{n-4} - \Delta^4 f_0\right)\right|.$$

Remark 1. It is worth noting that while the implied by (1.6) error estimate

$$|R[Q_n; f]| \le c_5(Q_n)\|f^{(5)}\|_{C[0,1]}$$

requires knowledge of the magnitude of the $C[0,1]$–norm of the integrand's derivative, the error bounds in Theorem 1(ii) and Corollary 1 in terms of finite diferences are easy to evaluate and may serve as a simple criteria for the number of nodes n needed to guarantee the evaluation of $I[f]$ with a prescribed tolerance. (Note however that these error bounds apply only for 5-positive or 5-negative integrands.) Let us also mention that, according to Corollary 1, the symmetrical (and hence not definite) quadrature formula $\hat{Q}_n$ has smaller error bound than the definite quadrature formulae Q_n and $\widetilde{Q}_n$.

The rest of the paper is organised as follows. Section 2 contains some preliminaries. In Section 2.1 we give some known facts about the Peano kernel representation of linear functionals, and prove a simple necessary condition for a quadrature formula to be positive definite. Some facts about Bernoulli polynomials and numbers and the Euler-MacLaurin summation formula are given in Section 2.2. In Sections 3 we present some formulae for numerical differentiation to be used for replacement of the derivatives occurring in the Euler-MacLaurin formula. The proof of Theorem 1 and Corollary 1 is given in Section 4.

2. PRELIMINARIES

2.1. PEANO KERNEL REPRESENTATION OF LINEAR FUNCTIONALS

For $r \in \mathbb{N}$, the Sobolev class of functions $W_1^r = W_1^r[0,1]$ is defined by

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

and contains, in particular, the class $C^r[0,1]$.

If $\mathcal{L}$ is a linear functional defined in $W_1^r[0,1]$ which vanishes on π_{r-1}, then, by a classical result of Peano [11], $\mathcal{L}$ is represented in the form

$$\mathcal{L}[f] = \int_0^1 K_r(t) f^{(r)}(t)\,dt\,,$$

where $K_r(t) = K_r(\mathcal{L}; t)$ is given by

$$K_r(t) = \mathcal{L}\Big[\frac{(\cdot - t)_+^{r-1}}{(r-1)!}\Big], \quad t \in [0,1]\,, \qquad u_+(t) = \max\{t, 0\}\,, \quad t \in \mathbb{R}\,.$$

When $\mathcal{L}$ is the remainder $R[Q;\cdot]$ of a quadrature formula Q with $ADP(Q) \geq r-1$, with some notational and language abuse, $K_r(t) = K_r(Q;t)$ is referred to as the r-th Peano kernel of Q. For Q as in (1.1), explicit representations for $K_r(Q;t)$, $t \in [0,1]$, are

$$K_r(Q;t) = \frac{(1-t)^r}{r!} - \frac{1}{(r-1)!}\sum_{i=0}^{n} a_i (x_i - t)_+^{r-1}, \tag{2.1}$$

and

$$K_r(Q;t) = (-1)^r \Big[\frac{t^r}{r!} - \frac{1}{(r-1)!}\sum_{i=0}^{n} a_i (t - x_i)_+^{r-1}\Big]. \tag{2.2}$$

Thus, for $f \in C^r[0,1]$ and a quadrature formula Q with $ADP(Q) = r-1$,

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

It is clear now that Q is a positive (negative) definite quadrature formula of order r if and only if $ADP(Q) = r-1$ and $K_r(Q;t) \geq 0$ (resp. $K_r(Q;t) \leq 0$) for all $t \in [0,1]$, and if this is the case, then

$$c_r(Q) = \int_0^1 K_r(Q;t)\, dt\,.$$

From (2.1) and (2.2) one easily derives the following necessary condition for positive (negative) definiteness of a quadrature formula.

Lemma 1. *Let*

$$Q[f] = \sum_{k=0}^{n} a_k\, f(x_k)\,, \quad 0 = x_0 < x_1 < \cdots < x_n = 1,$$

be a quadrature formula for $I[f] = \int_0^1 f(x)\,dx$. *A necessary condition for* Q *to be positive (resp., negative) definite of order* r *is*

$$(-1)^r a_0 \leq 0 \quad \textit{and} \quad a_n \leq 0 \quad (\textit{resp.},\ (-1)^r a_0 \geq 0 \quad \textit{and} \quad a_n \geq 0)\,.$$

Proof. If Q is positive or negative definite of order r, then $ADP(Q) = r-1$, and therefore $K_r(Q;t) \geq 0$ (resp., $K_r(Q;t) \leq 0$) for every $t \in (0,1)$. From (2.1) and (2.2) we find that for sufficiently small $\varepsilon > 0$

$$\operatorname{sign} K_r(Q; x_n - \varepsilon) = -\operatorname{sign} a_n\,, \quad \operatorname{sign} K_r(Q; x_0 + \varepsilon) = (-1)^{r+1} \operatorname{sign} a_0\,,$$

whence the conclusion follows. □

Assuming f is smooth enough, the remainder of the n-th compound trapezium quadrature formula

$$Q_n^{Tr}[f] = \frac{1}{2n}\big(f_0 + f_n\big) + \frac{1}{n}\sum_{k=1}^{n-1} f_k$$

(with $f_i = f(x_i)$ and $x_i = i/n$, $i = 0, \ldots, n$) admits an expansion of the form

$$R[Q_n^{Tr}; f] = -\sum_{\nu=1}^{[\frac{s}{2}]} \frac{B_{2\nu}(0)}{n^{2\nu}}\big[f^{(2\nu-1)}(1) - f^{(2\nu-1)}(0)\big] + \frac{(-1)^s}{n^s}\int_0^1 \widetilde{B}_s(nx) f^{(s)}(x)dx\,.$$

This is the so-called Euler-Maclaurin summation formula (see, e.g., [4, Satz 98]). Here, $\{B_\nu\}$ are the Bernoulli polynomials, which are defined recursively by

$$B_0(x) = 1, \quad B'_\nu(x) = B_{\nu-1}(x), \qquad \int_0^1 B_\nu(t)\,dt = 0\,, \qquad \nu \in \mathbb{N},$$

and $\widetilde{B}_\nu$ is the one-periodic extension of B_ν, i.e., $\widetilde{B}_\nu(x) = B_\nu(\{x\})$, where $\{x\}$ is the fractional part of $x \in \mathbb{R}$.

In the case $s = 5$ the Euler–Maclaurin summation formula reads as

$$\begin{aligned} I[f] =& Q_n^{Tr}[f] - \frac{1}{12n^2}\big[f'(1) - f'(0)\big] + \frac{1}{720n^4}\big[f'''(1) - f'''(0)\big] \\ & - \frac{1}{n^5}\int_0^1 \widetilde{B}_5(nx) f^{(5)}(x)\,dx\,, \end{aligned} \tag{2.3}$$

with the explicit form of B_5

$$B_5(x) = \frac{x^5}{120} - \frac{x^4}{48} + \frac{x^3}{72} - \frac{x}{720}\,.$$

Let us note that for $x \in \mathbb{R}$

$$-c \le \widetilde{B}_5(x) \le c\,, \qquad \text{where} \quad c := \frac{3+\sqrt{30}}{21600}\sqrt{1 - 2\sqrt{\frac{2}{15}}} \approx 0.000203818\,.$$

Rewriting (2.3) in the form

$$\begin{aligned} I[f] =& Q_n^{Tr}[f] - \frac{1}{12\,n^2}\big[f'(1) - f'(0)\big] + \frac{1}{720\,n^4}\big[f'''(1) - f'''(0)\big] \\ & - \frac{c}{n^5}\big[f^{(4)}(1) - f^{(4)}(0)\big] + \frac{1}{n^5}\int_0^1 \Big(c - \widetilde{B}_5(nx)\Big) f^{(5)}(x)\,dx\,, \end{aligned}$$

we observe that the quadrature formula

$$
\begin{aligned}
Q_n^*[f] =& Q_n^{Tr}[f] - \frac{1}{12\,n^2}\big[f'(x_n) - f'(x_0)\big] + \frac{1}{720\,n^4}\big[f'''(x_n) - f'''(x_0)\big] \\
&- \frac{c}{n^5}\big[f^{(4)}(x_n) - f^{(4)}(x_0)\big]
\end{aligned}
\tag{2.4}
$$

is positive definite of order 5, since

$$
K_5(Q_n^*;t) = n^{-5}\big(c - \widetilde{B}_5(nt)\big) \ge 0, \qquad t \in \mathbb{R}\,. \tag{2.5}
$$

However, Q_n^* is not of desired form, as it involves evaluations of both the integrand and of its derivatives. In order to obtain a quadrature formula using only integrand's evaluation, we need some formulae for numerical differentiation.

3. FORMULAE FOR NUMERICAL DIFFERENTIATION

The following formulae for numerical differentiation will be used to replace the derivatives occurring in quadrature formula Q_n^* (recall that $x_i = i/n$ and $f_i = f(x_i)$ for $i = 0, \dots, n$):

$$
\begin{aligned}
f'(x_0) &\approx D_1[f] := \frac{n}{12}\big[-25\,f_0 + 48\,f_1 - 36\,f_2 + 16\,f_3 - 3\,f_4\big]\,,\\
f'''(x_0) &\approx D_3[f] := \frac{n^3}{2}\big[-5\,f_0 + 18\,f_1 - 24\,f_2 + 14\,f_3 - 3\,f_4\big]\,,\\
f^{(4)}(x_0) &\approx D_4[f] := n^4\big[f_0 - 4\,f_1 + 6\,f_2 - 4\,f_3 + f_4\big] = n^4\Delta^4 f_0\,,
\end{aligned}
$$

$$
\begin{aligned}
f'(x_n) &\approx \widetilde{D}_1[f] := \frac{n}{12}\big[25\,f_n - 48\,f_{n-1} + 36\,f_{n-2} - 16\,f_{n-3} + 3\,f_{n-4}\big]\,,\\
f'''(x_n) &\approx \widetilde{D}_3[f] := \frac{n^3}{2}\big[5\,f_n - 18\,f_{n-1} + 24\,f_{n-2} - 14\,f_{n-3} + 3\,f_{n-4}\big]\,,\\
f^{(4)}(x_n) &\approx \widetilde{D}_4[f] := n^4\big[f_n - 4\,f_{n-1} + 6\,f_{n-2} - 4\,f_{n-3} + f_{n-4}\big] = n^4\Delta^4 f_{n-4}\,.
\end{aligned}
$$

These formulae are sharp for $f \in \pi_4$, i.e., the linear functionals

$$
L_j[f] := f^{(j)}(x_0) - D_j[f]\,,\quad \widetilde{L}_j[f] := f^{(j)}(x_n) - \widetilde{D}_j[f]\,,\quad j = 1,\,3,\,4
$$

vanish on π_4. According to Peano's theorem, for $f \in C^5[0,1]$ they admit integral representations, in particular,

$$
L_j[f] := \int_0^1 K_5(L_j;t)f^{(5)}(t)\,dt\,,\quad K_5(L_j;t) = L_j\Big[\frac{(\cdot - t)_+^4}{4!}\Big]\,,\quad j = 1,\,3,\,4\,. \tag{3.1}
$$

Proposition 2. *The Peano kernels* $K_5(L_j;\cdot)$, $j=1,3,4$, *vanish identically on the interval* $[x_4,x_n]$. *Moreover,*

$$\int_0^1 K_5(L_1;t)\,dt=\frac{1}{5n^4}\,, \tag{3.2}$$

$$\int_0^1 K_5(L_3;t)\,dt=\frac{7}{4n^2}\,, \tag{3.3}$$

$$\int_0^1 K_5(L_4;t)\,dt=-\frac{2}{n}\,. \tag{3.4}$$

Proof. The first claim follows from (3.1): for $t\ge x_4$ and $x\le x_4$ we have, by definition, $(x-t)_+^4\equiv 0$, hence $K_5(L_j;t)=L_j[(\cdot-t)_+^4]/4!\equiv 0$ for $t\in[x_4,x_n]$.

Equality (3.2) is verified as follows:

$$\begin{aligned}\int_0^1 K_5(L_1;t)\,dt&=-\frac{n}{288}\int_0^1\Big[48(x_1-t)_+^4-36(x_2-t)_+^4+16(x_3-t)_+^4-3(x_4-t)_+^4\Big]\,dt\\&=\frac{n}{1440}\Big[48(x_1-t)^5\Big|_0^{x_1}-36(x_2-t)^5\Big|_0^{x_2}+16(x_3-t)^5\Big|_0^{x_3}-3(x_4-t)^5\Big|_0^{x_4}\Big]\\&=\frac{1}{5n^4}\,.\end{aligned}$$

Equalities (3.3) and (3.4) are verified in the same way. □

In order to deduce an analogous statement for the linear functionals $\widetilde{L}_j$, we need a more convenient formula for their Peano kernels. Since

$$(x-t)_+^4+(t-x)_+^4=(x-t)^4 \quad \text{for every} \quad x,t\in\mathbb{R}\,,$$

and $\widetilde{L}_j$ vanish on π_4, it follows that $\widetilde{L}_j[(\cdot-t)_+^4]=-\widetilde{L}_j[(t-\cdot)_+^4]$, hence

$$\widetilde{L}_j[f]:=\int_0^1 K_5(\widetilde{L}_j;t)f^{(5)}(t)\,dt\,,\quad K_5(\widetilde{L}_j;t)=-\widetilde{L}_j\Big[\frac{(t-\cdot)_+^4}{4!}\Big]\,,\quad j=1,\,3,\,4\,. \tag{3.5}$$

By using (3.5), we establish in the same manner the following:

Proposition 3. *The Peano kernels* $K_5(\widetilde{L}_j;\cdot)$, $j=1,3,4$, *vanish identically on the interval* $[x_0,x_{n-4}]$. *Moreover,*

$$\int_0^1 K_5(\widetilde{L}_1;t)\,dt=\frac{1}{5n^4}\,,$$

$$\int_0^1 K_5(\widetilde{L}_3;t)\,dt=\frac{7}{4n^2}\,,$$

$$\int_0^1 K_5(\widetilde{L}_4;t)\,dt=\frac{2}{n}\,.$$

4. PROOF OF THEOREM 1

Replacement of the derivatives in (2.4) with the formulae for numerical differentiation from Section 3 yields

$$\begin{aligned}Q_n^*[f] =&Q_n^{Tr}[f] + \frac{D_1[f]}{12n^2} - \frac{D_3[f]}{720n^4} + c\,\frac{D_4[f]}{n^5} - \frac{\widetilde{D}_1[f]}{12n^2} + \frac{\widetilde{D}_3[f]}{720n^4} - c\,\frac{\widetilde{D}_4[f]}{n^5}\\ &+\frac{1}{12n^2}\big(L_1[f]-\widetilde{L}_1[f]\big)-\frac{1}{720n^4}\big(L_3[f]-\widetilde{L}_3[f]\big)+\frac{c}{n^5}\big(L_4[f]-\widetilde{L}_4[f]\big)\\ =:&\widehat{Q}_n[f] + L[f]\,,\end{aligned} \tag{4.1}$$

where the linear functional L is given by

$$L = \frac{1}{12n^2}\,\big(L_1 - \widetilde{L}_1\big) - \frac{1}{720n^4}\,\big(L_3 - \widetilde{L}_3\big) + \frac{c}{n^5}\big(L_4 - \widetilde{L}_4\big) \tag{4.2}$$

and $\widehat{Q}_n$ is the quadrature formula

$$\widehat{Q}_n[f] = \frac{1}{n}\sum_{k=0}^{n} a_k\, f_k + \frac{c}{n}\,\big(\Delta^4 f_0 - \Delta^4 f_{n-4}\big) \tag{4.3}$$

with coefficients

$$\begin{aligned}&a_0 = a_n = \frac{95}{288}, \quad a_1 = a_{n-1} = \frac{317}{240}, \quad a_2 = a_{n-2} = \frac{23}{30},\\ &a_3 = a_{n-3} = \frac{793}{720}, \quad a_4 = a_{n-4} = \frac{157}{160}\,, \quad a_k = 1, \quad 5 \le k \le n-5\,.\end{aligned} \tag{4.4}$$

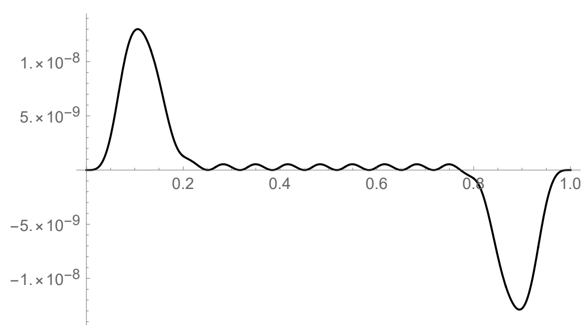


Figure 1. The graph of $K_5(\widehat{Q}_n;t)$, $n = 15$.

Clearly, $ADP(\widehat{Q}_n) \ge 4$. Unfortunately, $\widehat{Q}_n$ is not positive definite of order 5, as $K_5(\widehat{Q}_n;t)$ is negative in a neighborhood of $x_n = 1$, see Figure 1. In fact, $\widehat{Q}_n$ fails to satisfy the criteria for positive definiteness of Lemma 1, as the coefficient of $f_n = f(x_n)$ in $\widehat{Q}_n$ is

$$\kappa = \frac{1}{n}\Big(\frac{95}{288} - c\Big) > 0\,.$$

In order to fulfill the necessary condition for positive definiteness of Lemma 1, we modify $\widehat{Q}_n$ so that the coefficient of $f(x_n)$ equals zero:

$$\begin{aligned} Q_n[f] &= \widehat{Q}_n[f] - \kappa\, L_5[f]\,, &\quad (4.5)\\ L_5[f] &= -f_{n-5} + 5\,f_{n-4} - 10\,f_{n-3} + 10\,f_{n-2} - 5\,f_{n-1} + f_n\,. &\quad (4.6)\end{aligned}$$

Since the finite difference functional $L_5[f] = \Delta^5 f_{n-5}$ vanishes on π_4, the newly built quadrature formula Q_n uses the equispaced nodes and $ADP(Q_n) = 4$. Assuming $n \geq 11$ and using (4.3), (4.4), (4.5) and (4.6), we find that

$$Q_n[f] = \frac{1}{n}\sum_{k=0}^{n-1} A_k\, f_k + \frac{c}{n}\left(\Delta^4 f_0 - \Delta^4 f_{n-5}\right),$$

where $A_k = 1$ for $5 \leq k \leq n-6$ and

$$A_0 = \frac{95}{288},\quad A_1 = \frac{317}{240},\quad A_2 = \frac{23}{30},\quad A_3 = \frac{793}{720},\quad A_4 = \frac{157}{160},$$

$$A_{n-5} = \frac{383}{288},\quad A_{n-4} = -\frac{481}{720},\quad A_{n-3} = \frac{22}{5},\quad A_{n-2} = -\frac{1823}{720},\quad A_{n-1} = \frac{4277}{1440}\,.$$

Hence, Q_n is the quadrature formula from Theorem 1.

We need to show that Q_n is positive definite of order 5, i.e. that $K_5(Q_n;t) \geq 0$ for $t \in (0,1)$. To this end, we observe that, by virtue of (4.1) and (4.2),

$$Q_n = Q_n^* - L - \kappa\, L_5$$

with L and L_5 given by (4.2) and (4.6), respectively. Consequently,

$$K_5(Q_n;t) = K_5(Q_n^*;t) + K_5(L;t) + \kappa K_5(L_5;t)\,. \qquad (4.7)$$

According to (2.5), $K_5(Q_n^*;t) \geq 0$ for $t \in (0,1)$. From (4.2) and Propositions 2 and 3 we infer that

$$K_5(L;t) \equiv 0 \quad \text{for} \quad t \in [x_4, x_{n-4}]\,. \qquad (4.8)$$

A similar conclusion is true for $K_5(L_5;t)$, as it is a B-spline of degree 4 with knots x_i, $n-5 \leq i \leq n$, and therefore

$$K_5(L_5;t) \equiv 0 \quad \text{for} \quad t \in [x_0, x_{n-5}]\,. \qquad (4.9)$$

It follows from (4.7), (2.5), (4.8) and (4.9) that $K_5(Q_n;t) \equiv K_5(Q_n^*;t) \geq 0$ on the interval $[x_4, x_{n-5}]$, therefore we only need to verify that $K_5(Q_n;t) \geq 0$ in the cases $t \in (x_0, x_4)$ and $t \in (x_{n-5}, x_n)$.

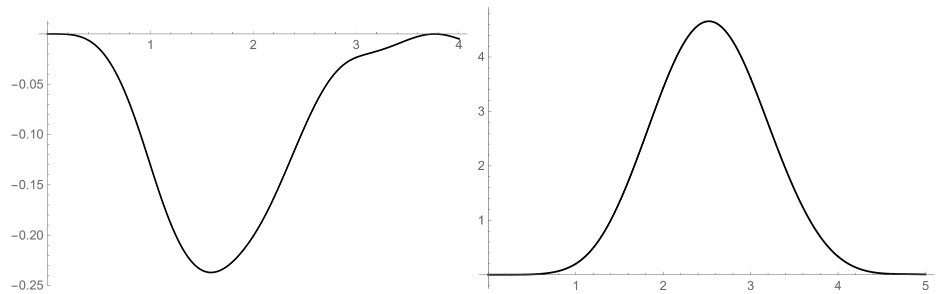
Case 1: $t \in (x_0, x_4)$. By the change of variable $t = u/n$, $u \in (0,4)$, we obtain

$$K_5(Q_n;t) = -\frac{1}{4!\,n^5}\,\varphi_1(u)\,, \quad u \in (0,4)\,,$$

where the function φ_1 does not depend on n, namely,

$$\varphi_1(u) = \frac{u^5}{5} - (A_0 + c)u^4 - (A_1 - 4c)(u-1)_+^4 - (A_2 + 6c)(u-2)_+^4 - (A_3 - 4c)(u-3)_+^4 .$$

The graph of φ_1, depicted in Figure 2(a), shows that $\varphi_1(u) < 0$ in the interval $(0,4)$ (φ_1 has a local maximum at $u = 3.76475$, equal to -0.000059). Therefore, $K_5(Q_n;t) > 0$ for $t \in (x_0, x_4)$.



(a) The graph of $\varphi_1(u)$, $0 \le u \le 4$.

(b) The graph of $\varphi_2(u)$, $0 \le u \le 5$.

Figure 2

Case 2: $t \in (x_{n-5}, x_n)$. By the change of variable $t = 1 - u/n$ we obtain

$$K_5(Q_n;t) = \frac{1}{4!\, n^5}\, \varphi_2(u)\,, \quad u \in (0,5)\,,$$

where

$$\varphi_2(u) = \frac{u^5}{5} - B_1(u-1)_+^4 - B_2(u-2)_+^4 - B_3(u-3)_+^4 - B_4(u-4)_+^4\,,$$

with $B_i = A_{n-i} + (-1)^i \binom{4}{i-1} c$, $i = 1, \ldots, 5$. Again, φ_2 does not depend on n and is positive for $u \in (0,5)$, as shown in Figure 2(b). Consequently, $K_5(Q_n;t) > 0$ for $t \in (x_{n-5}, x_n)$, and the proof that Q_n is a positive definite quadrature formula of order 5 is completed.

Having established the positive definiteness of Q_n, we proceed with evaluating its error constant $c_5(Q_n) = I[K_5(Q_n;\cdot)]$. From (4.7) we have

$$c_5(Q_n) = \int_0^1 K_5(Q_n^*;t)\,dt + \int_0^1 K_5(L;t)\,dt + \kappa \int_0^1 K_5(L_5;t)\,dt\,. \qquad (4.10)$$

We evaluate the three integrals on the right-hand side of (4.10). For the first one, we find from (2.5)

$$\int_0^1 K_5(Q_n^*;t)\,dt = \frac{1}{n^5} \int_0^1 \left(c - \widetilde{B}_5(nt)\right) dt = \frac{c}{n^5}\,.$$

According to (4.2),

$$\begin{aligned}K_5(L;t) =&\frac{1}{12n^2}\left(K_5(L_1;t)-K_5(\widetilde{L}_1;t)\right)-\frac{1}{720n^4}\left(K_5(L_3;t)-K_5(\widetilde{L}_3;t)\right)\\&+\frac{c}{n^5}\left(K_5(L_4;t)-K_5(\widetilde{L}_4;t)\right)\end{aligned}$$

and using Propositions 2 and 3, we obtain

$$\int_0^1 K_5(L;t)\,dt=-\frac{4c}{n^6}\,.$$

Recall that $L_5[f]=\Delta^5 f_{n-5}$, and from Peano's representation theorem,

$$\begin{aligned}K_5(L_5;t)=\frac{1}{4!}\big[&(x_n-t)_+^4-5(x_{n-1}-t)_+^4+10(x_{n-2}-t)_+^4\\&-10(x_{n-3}-t)_+^4+5(x_{n-4}-t)_+^4-(x_{n-5}-t)_+^4\big]\,.\end{aligned}$$

Hence,

$$\begin{aligned}\int_0^1 K_5(L_5;t)\,dt&=\frac{1}{5!n^5}\left[n^5-5(n-1)^5+10(n-2)^5-10(n-3)^5+5(n-4)^5-(n-5)^5\right]\\&=\frac{1}{n^5}\,.\end{aligned}$$

Substituting the found values of the three integrals in (4.10), we obtain

$$c_5(Q_n)=\frac{c}{n^5}-\frac{4c}{n^6}+\frac{1}{n^6}\Big(\frac{95}{288}-c\Big)=\frac{c}{n^5}+\frac{5(19-288c)}{288n^6}\,,$$

which was to be proved. This accomplishes the proof of Theorem 1(i).

For the proof of Theorem 1(ii) we apply Proposition 1(ii). We set $A_n=0$, hence Q_n becomes a nodes-symmetrical quadrature formula. Now, according to (1.5),

$$B(Q_n;f)=\big|\widetilde{Q}_n[f]-Q_n[f]\big|=\big|Q_n[\widetilde{f}]-Q_n[f]\big|\,,\qquad\text{where}\quad\widetilde{f}(t)=f(1-t)\,.$$

In view of (4.3) and (4.5),

$$Q_n[f]=\frac{1}{n}\sum_{k=0}^{n}a_k\,f_k+\frac{c}{n}\left(\Delta^4 f_0-\Delta^4 f_{n-4}\right)-\kappa\,\Delta^5 f_{n-5}\,.$$

Making use of relations $\Delta^4\widetilde{f}_0=\Delta^4 f_{n-4}$, $\Delta^4\widetilde{f}_{n-4}=\Delta^4 f_0$, $\Delta^5\widetilde{f}_{n-5}=-\Delta^5 f_0$ and $a_k=a_{n-k}$, $k=0,\dots,n$ (see (4.2)), we obtain

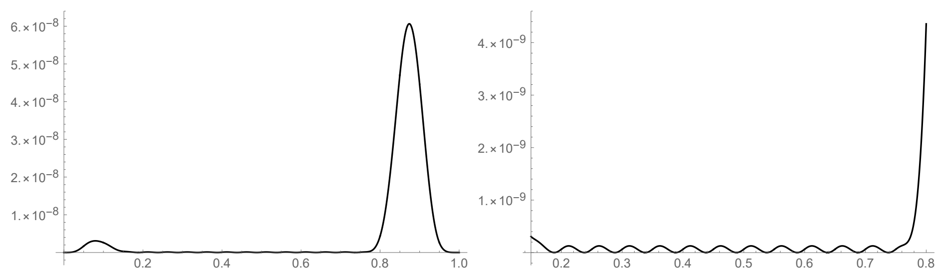
$$Q_n[\widetilde{f}]=\frac{1}{n}\sum_{k=0}^{n}a_k\,f_k+\frac{c}{n}\left(\Delta^4 f_{n-4}-\Delta^4 f_0\right)+\kappa\,\Delta^5 f_0\,.$$

Hence,

$$B(Q_n;f) = \left|Q_n[\widetilde{f}] - Q_n[f]\right| = \left|\kappa\left(\Delta^5 f_0 + \Delta^5 f_{n-5}\right) + \frac{2c}{n}\left(\Delta^4 f_{n-4} - \Delta^4 f_0\right)\right|$$
$$= \frac{1}{n}\left|\Big(\frac{95}{288} - c\Big)\left(\Delta^5 f_0 + \Delta^5 f_{n-5}\right) + 2c\left(\Delta^4 f_{n-4} - \Delta^4 f_0\right)\right|.$$

Claim (ii) of Theorem 1 now follows from Proposition 1(ii). The proof of Theorem 1 is completed. Corollary 1 is a consequence of Theorem 1 and Proposition 1.

Remark 2. The magnitude of the Peano kernel $K_5(Q_n;t)$ in the interval $[x_4, x_{n-5}]$ is much smaller compared to its magnitude near the endpoints of $(0,1)$, see Figure 3. A further perturbation of Q_n of the form $Q_n'[f] = Q_n[f] + \kappa_1\,\Delta^5 f_0$ is possible, with $\kappa_1 > 0$ small enough so that $0 \le K_5(Q_n';t) < K_5(Q_n;t)$ in (x_0, x_5). Eventually, this leads to a quadrature formula Q_n' which is positive definite of order 5 and has a slightly smaller error constant, $c_5(Q_n') < c_5(Q_n)$. The improvement however is negligible, so we decided not to perform this step.



(a) Graph of $K_5(Q_n;t)$, $t \in [0,1]$. (b) Graph of $K_5(Q_n;t)$, $t \in [x_3, x_{n-4}]$.

Figure 3: Graphs of $K_5(Q_n;t)$, $n = 20$.

ACKNOWLEDGEMENT. The authors were supported by the Sofia University Research Fund through Contract No. 80-10-17/09.04.2019. The first author was supported of the Bulgarian Ministry of Education and Science under the National Research Programme “Young scientists and postdoctoral students” approved by DCM No. 577/17.08.2018.

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Received on December 17, 2019

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