ГОДИШНИК НА СОФИЙСКИЯ УНИВЕРСИТЕТ „СВ. КЛИМЕНТ ОХРИДСКИ“

ФАКУЛТЕТ ПО МАТЕМАТИКА И ИНФОРМАТИКА
Том 104

ANNUAL OF SOFIA UNIVERSITY „ST. KLIMENT OHRIDSKI“

FACULTY OF MATHEMATICS AND INFORMATICS
Volume 104

DEFINITE QUADRATURE FORMULAE OF ORDER THREE WITH EQUIDISTANT NODES

ANA AVDZHIEVA, VESSELIN GUSHEV, GENO NIKOLOV

A sequence of definite quadrature formulae of order three with equidistant nodes is constructed. The error constants of these quadratures are evaluated and simple a posteriori error estimates derived under the assumption that the integrand's third 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

For the purposes of numerical integration, the definite integral

$$I[f] := \int_0^1 f(x)\,dx \tag{1.1}$$

is approximated by a quadrature formula, i.e., a linear functional of the form

$$Q[f] = \sum_{i=0}^{n} a_i\, f(x_i), \qquad 0 \le x_0 < x_1 < \cdots < x_n \le 1\,. \tag{1.2}$$

Quadrature formula (1.2) 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 algebraic polynomials of degree not exceeding k.

We are interested in definite quadrature formulae.

Definition 1. Quadrature formula (1.2) 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 $c_r(Q) > 0$ ($c_r(Q) < 0$).

The importance of the definite quadrature formulae of order r stems in the fact that they provide one-sided approximation to $I[f]$ whenever $f^{(r)}$ has a permanent sign in the integration interval. For brevity sake, we adopt the following

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 $x \in [0, 1]$.

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 for the true value of $I[f]$ we have the inclusion $Q^+[f] \leq I[f] \leq Q^-[f]$. This simple observation serves as a base for 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 of quadratures used in practice (e.g., quadrature formulae of Gauss, Radau, Lobatto, Newton-Cotes) are definite of certain order.

Perhaps, the best known definite quadrature formulae are the midpoint and the trapezium rules,

$$Q_n^{Mi}[f] = \frac{1}{n}\sum_{k=1}^{n} f\Big(\frac{2k-1}{2n}\Big), \qquad Q_{n+1}^{Tr}[f] = \frac{1}{2n}\big(f(0) + f(1)\big) + \frac{1}{n}\sum_{k=1}^{n-1} f\Big(\frac{k}{n}\Big),$$

they are respectively positive and negative definite of order two. Moreover, Q_n^{Mi} and Q_{n+1}^{Tr} are the optimal definite quadrature formulae of order two. The latter means that $c_2(Q_n^{Mi}) = \frac{1}{24n^2}$ is the smallest possible error constant of a n-point positive definite quadrature formula of order two, and $c_2(Q_{n+1}^{Tr}) = -\frac{1}{12n^2}$ is the largest possible error constant of a $(n+1)$-point negative definite quadrature formulae of order two. Additional advantages of Q_n^{Mi} and Q_{n+1}^{Tr} are that they use equispaced nodes and equal weights.

The optimal definite quadrature formulae of higher order are not known explicitly, although their existence and uniqueness is known, see [10, 4, 6, 7]. In [10] Schmeisser [10] constructed optimal definite quadrature formulae of even order *with equidistant nodes.* Köhler and Nikolov [5] showed that certain Gauss-type quadratures for spaces of polynomial splines with double equidistant knots are asymptotically optimal definite quadrature formulae, and based on this result, Nikolov [8] proposed an algorithm for the construction of asymptotically optimal definite quadrature formulae of order four. In a recent paper [1] two of the authors constructed sequences of asymptotically optimal definite quadrature formulae of order four with all but few boundary nodes being equidistant; moreover, for suitable pairs of such definite quadrature formulae they derived a posteriori error estimates.

The simplest example of a pair of definite quadrature formulae of odd order is the left- and the right- rectangle rules,

$$Q_+[f] = \frac{1}{n}\sum_{k=0}^{n-1} f\Big(\frac{k}{n}\Big), \qquad Q_-[f] = \frac{1}{n}\sum_{k=1}^{n} f\Big(\frac{k}{n}\Big),$$

which are a positive and a negative definite quadrature formula, respectively, of order one. Indeed, if f is an $1-$positive (or simply nondecreasing) function, then $R[Q_+;f] \geq 0$, $R[Q_-;f] \leq 0$, and

$$|R[Q_\pm[f]| \leq Q_-[f] - Q_+[f] = \frac{1}{n}\big(f(1) - f(0)\big). \tag{1.3}$$

We observe some differences with the definite quadrature formulae of even order: while, most often, definite quadrature formulae of even order are symmetrical, the left and the right rectangles formulae are non-symmetrical. Furthermore, each of them is obtained from the other one by a *reflection.*

Definition 3. Quadrature formula (1.2) is called:

- *symmetrical*, if

$$a_k = a_{n-k}\,, \qquad k = 0, \dots, n\,; \tag{1.4}$$

$$x_k = 1 - x_{n-k}\,, \qquad k = 0, \dots, n\,; \tag{1.5}$$

- *nodes-symmetrical*, if only condition (1.5) is satisfied;
- Quadrature formula

$$\widetilde{Q}[f] = \widetilde{Q}[Q;f] := \sum_{k=0}^{n} a_k\, f(x_{n-k}) \tag{1.6}$$

is called the *reflected quadrature formula* to (1.2).

Thus, a quadrature formula Q is symmetrical if and only if it coincides with its reflected, $\widetilde{Q}$. By adding (if necessary) nodes with weights equal to zero, each quadrature formula may be considered as nodes-symmetrical.

The following simple statement shows that our observations about the left- and the right- rectangle rules apply to a more general situation.

Proposition 1. *(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,*

$$c_r(\widetilde{Q}) = -c_r(Q)\,. \tag{1.7}$$

(ii) If Q is a nodes-symmetrical definite quadrature formula 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

$$\big|R[Q^*;f]\big| \le B[Q;f] := \left|\sum_{k=0}^{\lfloor \frac{n}{2}\rfloor}\big(a_k - a_{n-k}\big)\big(f(x_{n-k}) - f(x_k)\big)\right|. \tag{1.8}$$

(iii) Under the same assumptions for Q and f as in (ii), for the remainder of quadrature formula $\hat{Q} = \frac{1}{2}\,(Q+\widetilde{Q})$ we have

$$\big|R[\hat{Q};f]\big| \le \frac{1}{2}\,B[Q;f]\,. \tag{1.9}$$

Proof. (i) Let $\widetilde{f}(x) = f(1-x)$, then $I[f] = I[\widetilde{f}]$. If Q is a definite quadrature formula of order r, r - odd, and f is an $r-$positive or $r-$negative function, then $\widetilde{Q}[f] = Q[\widetilde{f}]$ and

$$R[\widetilde{Q};f] = I[f] - \widetilde{Q}[f] = I[\widetilde{f}] - Q[\widetilde{f}] = c_r(Q)\widetilde{f}^{(r)}(\xi) = -c_r(Q)f^{(r)}(1-\xi)\,,$$

which shows that $\widetilde{Q}$ is also definite of order r and $c_r(\widetilde{Q}) = -c_r(Q)$.

Now we prove (ii) and (iii). If, e.g., Q is a nodes-symmetrical positive definite quadrature formulae of order r and f is an $r-$positive function, then

$$Q[f] \le I[f] \le \widetilde{Q}[f]\,, \tag{1.10}$$

and consequently

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

Inequality (1.9) is an obvious consequence of (1.10). The proof of the other cases is completely analogous, and therefore is omitted. □

Proposition 1 implies, in particular, that definite quadrature formulae of odd order are never symmetrical. The error estimate (1.8) is especially simple when Q is of almost Chebyshev type, i.e. almost all weights of Q are equal to each other. The definite quadrature formulae constructed in this paper enjoy this property.

Before formulating our main result, let us introduce some notation.

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

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

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

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

Theorem 1. *For every $n \ge 8$, quadrature formula*

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

with coefficients $A_{k,n} = \frac{1}{n}$, $3 \le k \le n-4$, 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 3 with the error constant

$$c_3(Q_n) = \frac{\sqrt{3}}{216n^3} + \frac{27-\sqrt{3}}{72n^4}\,. \tag{1.11}$$

If f is a 3-positive or 3-negative function, then

$$\big|R[Q_n;f]\big| \le \frac{1}{216n}\,\big|81\big(\Delta^3 f_{n-3} - \Delta^3 f_0\big) + \sqrt{3}\big(\Delta^2 f_{n-2} + \Delta^2 f_{n-3} - \Delta^2 f_0 - \Delta^2 f_1\big)\big|\,.$$

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

Corollary 1. *The reflected to Q_n quadrature formula $\widetilde{Q}_n$ is negative definite of order 3 with the error constant $c_3(\widetilde{Q}_n) = -c_3(Q_n)$.*

If f is a 3-positive or 3-negative function and $\hat{Q}_n = \frac{1}{2}\big(Q_n + \widetilde{Q}_n\big)$, then

$$\big|R[\widetilde{Q}_n;f]\big| \le \frac{1}{216n}\,\big|81\big(\Delta^3 f_{n-3} - \Delta^3 f_0\big) + \sqrt{3}\big(\Delta^2 f_{n-2} + \Delta^2 f_{n-3} - \Delta^2 f_0 - \Delta^2 f_1\big)\big|\,,$$

$$\big|R[\hat{Q}_n;f]\big| \le \frac{1}{432n}\,\big|81\big(\Delta^3 f_{n-3} - \Delta^3 f_0\big) + \sqrt{3}\big(\Delta^2 f_{n-2} + \Delta^2 f_{n-3} - \Delta^2 f_0 - \Delta^2 f_1\big)\big|\,.$$

Let us point out that, while error estimates of the form

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

and alike require knowledge about the magnitude of integrand's derivative, the bounds in Theorem 1 and Corollary 1 in terms of finite differences involve only eight values of the integrand 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. In this respect, it is preferable to use quadrature formula $\hat{Q}_n$ rather than the definite quadrature formulae Q_n and $\widetilde{Q}_n$.

The rest of the paper is organised as follows. Section 2 provides known facts about the Peano kernel representation of linear functionals and the Euler-MacLaurin expansion formula for the remainder of the trapezium quadrature formula. In Sections 3 we present the proof of Theorem 1. In our construction of quadrature formula (1.10) we perform some optimization, minimizing its error constant and at the same time trying to preserve its almost Chebyshev structure.

2. PRELIMINARIES

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

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

In particular, $W_1^r[0,1]$ contains the class $C^r[0,1]$.

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

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

where

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

In the case when $\mathcal{L}$ is the remainder $R[Q;\cdot]$ of a quadrature formula Q with $ADP(Q) \ge r-1$, the function $K_r(t) = K_r(Q;t)$ is referred to as the r-th Peano kernel of Q. For Q as in (2.1), explicit representations for $K_r(Q;t)$, $t \in [0,1]$, are

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

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

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

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

it is clear that Q is a positive (negative) definite quadrature formula of order r if and only if $ADP(Q) = r-1$ and $K_r(Q;t) \ge 0$ (resp. $K_r(Q;t) \le 0$) for all $t \in [0,1]$.

Throughout this paper, $\{x_{k,n}\}_{k=0}^{n}$ will stand for the nodes of the n-th compound trapezium formula Q_{n+1}^{Tr},

$$x_{k,n} = \frac{k}{n}, \quad k = 0,\dots,n\,,$$

so that

$$Q_{n+1}^{Tr}[f] = \frac{1}{2n}\big(f(x_{0,n}) + f(x_{n,n})\big) + \frac{1}{n}\sum_{k=1}^{n-1} f(x_{k,n})\,. \tag{2.3}$$

Our definite quadrature formulae are obtained by an appropriate modification of Q_{n+1}^{Tr}. The following lemma gives a particular case of the Euler-Maclaurin formula, see, e.g., [2, Satz 98]:

Lemma 1. *Assume that $f \in W_1^3$. Then*

$$I[f] = Q_{n+1}^{Tr}[f] - \frac{1}{12n^2}\left[f'(1) - f'(0)\right] - \frac{1}{n^3}\int_0^1 \widetilde{B}_3(nx) f'''(x)\, dx\,, \tag{2.4}$$

where $\widetilde{B}_3$ is the 1-periodic extension of the third Bernoulli polynomial

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

Note that $\widetilde{B}_3(x) = B_3(\{x\})$, $x \in \mathbb{R}$, where $\{x\}$ stands for the fractional part of x. In the sequel, we shall use the fact that

$$-\frac{\sqrt{3}}{216} \le \widetilde{B}_3(x) \le \frac{\sqrt{3}}{216}\,, \qquad x \in \mathbb{R}\,. \tag{2.5}$$

3. PROOF OF THE RESULTS.

We rewrite formula (2.4) in Lemma 1 in the following form:

$$\begin{aligned} I[f] =& Q_{n+1}^{Tr}[f] - \frac{1}{12\,n^2}\left[f'(1) - f'(0)\right] - \frac{\sqrt{3}}{216\,n^3}\left[f''(1) - f''(0)\right] \\ &+ \frac{1}{n^3}\int_0^1 \Big(\frac{\sqrt{3}}{216} - \widetilde{B}_3(nx)\Big) f^{(3)}(x)\, dx \\ =:& \widetilde{Q}[f] + R[\widetilde{Q};f]\,, \end{aligned} \tag{3.1}$$

where

$$\widetilde{Q}[f] = Q_{n+1}^{Tr}[f] + \frac{1}{12n^2}f'(0) + \frac{\sqrt{3}}{216n^3}f''(0) - \frac{1}{12n^2}f'(1) - \frac{\sqrt{3}}{216n^3}f''(1)\,. \tag{3.2}$$

By (3.1) and (2.5) it follows that $\widetilde{Q}$ is a positive definite quadrature formula, however, it is not of the desired form as it involves values of integrand's derivatives. That is why we approximate the derivatives values at the end-points appearing in $\widetilde{Q}$ by pairs of formulae for numerical differentiation involving values at the closest nodes. The reason for not using single formulae for numerical differentiation is that it is not a priory clear whether they will result in a positive definite quadrature formula, so we need some flexibility to achieve definiteness.

Thus, $f'(0)$ is approximated as follows:

$$f'(0) \approx \frac{n}{2}\big[-3f(x_{0,n}) + 4f(x_{1,n}) + f(x_{2,n}) =: D_{1,1}[f]\,,$$

$$f'(0) \approx \frac{n}{2}\big[-5f(x_{1,n}) + 8f(x_{2,n}) - 3f(x_{3,n}) =: D_{1,2}[f]\,,$$

and for any $\alpha \in \mathbb{R}$ we have

$$\begin{aligned} &f'(0) \approx \alpha D_{1,1}[f] + (1-\alpha)D_{1,2}[f] =: D_1^{\alpha}[f]\,,\\ &L_1[f] := f'(0) - D_1^{\alpha}[f] \ \text{ vanishes on } \ \pi_2\,. \end{aligned} \tag{3.3}$$

Likewise, $f''(0)$ is approximated by

$$f''(0) \approx n^2\big[f(x_{0,n}) - 2f(x_{1,n}) + f(x_{2,n}) =: D_{2,1}[f]\,,$$

$$f''(0) \approx n^2\big[f(x_{1,n}) - 2f(x_{2,n}) + f(x_{3,n}) =: D_{2,2}[f]\,,$$

and for any $\beta \in \mathbb{R}$

$$\begin{aligned} &f''(0) \approx \beta D_{2,1}[f] + (1-\beta)D_{2,2}[f] =: D_2^{\beta}[f]\,,\\ &L_2[f] := f''(0) - D_2^{\beta}[f] \ \text{ vanishes on } \ \pi_2\,. \end{aligned} \tag{3.4}$$

For the approximation of $f'(1)$ and $f''(1)$ we use the above formulae for numerical differentiation, applied to $-f(1-x)$ and $f(1-x)$, respectively. For the first derivative this yields

$$f'(1) \approx \frac{n}{2}\big[3f(x_{n,n}) - 4f(x_{n-1,n}) - f(x_{n-2,n}) =: \widetilde{D}_{1,1}[f]\,,$$

$$f'(1) \approx \frac{n}{2}\big[5f(x_{n-1,n}) - 8f(x_{n-2,n}) + 3f(x_{n-3,n}) =: \widetilde{D}_{1,2}[f]\,,$$

and for any $\gamma \in \mathbb{R}$ we have

$$\begin{aligned} &f'(1) \approx \gamma\widetilde{D}_{1,1}[f] + (1-\gamma)D_{1,2}[f] =: \widetilde{D}_1^{\gamma}[f]\,,\\ &\widetilde{L}_1[f] := f'(1) - \widetilde{D}_1^{\gamma}[f] \ \text{ vanishes on } \ \pi_2\,. \end{aligned} \tag{3.5}$$

Similarly,

$$f''(1) \approx n^2 \left[f(x_{n,n}) - 2f(x_{n-1,n}) + f(x_{n-2,n}) =: \widetilde{D}_{2,1}[f] \right.,$$

$$f''(1) \approx n^2 \left[f(x_{n-1,n}) - 2f(x_{n-2,n}) + f(x_{n3,n}) =: \widetilde{D}_{2,2}[f] \right.,$$

and for any $\delta \in \mathbb{R}$

$$\begin{aligned} &f''(1) \approx \delta \widetilde{D}_{2,1}[f] + (1-\delta)\widetilde{D}_{2,2}[f] =: \widetilde{D}_2^{\delta}[f]\,, \\ &\widetilde{L}_2[f] := f''(1) - \widetilde{D}_2^{\delta}[f] \ \text{ vanishes on } \ \pi_2\,. \end{aligned} \tag{3.6}$$

The replacement of $f'(0)$, $f''(0)$, $f'(1)$ and $f''(1)$ in (3.2) by $D_1^{\alpha}[f]$, $D_2^{\beta}[f]$, $\widetilde{D}_1^{\gamma}[f]$ and $\widetilde{D}_2^{\delta}[f]$, respectively, yields a quadrature formula

$$Q[f] = \sum_{k=0}^{n} A_{k,n} f\Big(\frac{k}{n}\Big)\,, \tag{3.7}$$

which, by construction, evaluates $I[f]$ to the exact value whenever $f \in \pi_2$.

Assuming that $n \geq 8$, we have $A_{k,n} = 1/n$ for $4 \leq k \leq n-4$. Formally, coefficients $A_{k,n}$, $0 \leq k \leq 3$, depend on parameters α and β, while coefficients $A_{k,n}$, $n-3 \leq k \leq n$ depend on parameters γ and δ. In fact, it is not difficult to see that $\{A_{k,n}\}_0^3$ depend on a single parameter, say θ, while $\{A_{k,n}\}_{n-3}^n$ depend on another single parameter, say ϱ, where

$$\theta := 27\alpha - \sqrt{3}\beta\,, \qquad \varrho := 27\gamma + \sqrt{3}\delta\,.$$

Specifically, we have

$$\begin{aligned} A_{0,n} &= \frac{108-\theta}{216n}, & A_{1,n} &= \frac{171+\sqrt{3}+3\theta}{216n}, \\ A_{2,n} &= \frac{288-2\sqrt{3}-3\theta}{216n}, & A_{3,n} &= \frac{189+\sqrt{3}+\theta}{216n}, \\ A_{n-3,n} &= \frac{189-\sqrt{3}+\varrho}{216n}, & A_{n-2,n} &= \frac{288+2\sqrt{3}-3\varrho}{216n}, \\ A_{n-1,n} &= \frac{171-\sqrt{3}+3\varrho}{216n}, & A_{n,n} &= \frac{108-\varrho}{216n}\,, \\ A_{k,n} &= \frac{1}{n}, \quad 4 \leq k \leq n-4. \end{aligned}$$

Our next goal is to determine the values of parameters θ and ϱ which ensure that quadrature formula (3.7) is positive definite of order 3. Not only want we (3.7) to be positive definite, but also require θ and ϱ to be chosen in such a way that its error constant, $c_3(Q)$, is as small as possible. To this end, let us look closer at the third Peano kernel of Q.

From (3.2)–(3.6) we observe that

$$R[Q;f]=R[\widetilde{Q};f]+\frac{1}{12n^2}\,L_1[f]+\frac{\sqrt{3}}{216n^3}\,L_2[f]+\frac{1}{12n^2}\,\widetilde{L}_1[f]+\frac{\sqrt{3}}{216n^3}\,\widetilde{L}_2[f]\,,$$

therefore

$$\begin{aligned}K_3(Q;t)=K_3(\widetilde{Q};t)&+\frac{1}{12n^2}\,K_3(L_1;t)+\frac{\sqrt{3}}{216n^3}\,K_3(L_2;t)\\&+\frac{1}{12n^2}\,K_3(\widetilde{L}_1;t)+\frac{\sqrt{3}}{216n^3}\,K_3(\widetilde{L}_2;t)\,.\end{aligned}\tag{3.8}$$

Based on the definition of Peano kernels, it is not difficult to see that $K_3(L_1;\cdot)$ and $K_3(L_2;\cdot)$ vanish identically on the interval $[x_{3,n},1]$ whereas $K_3(\widetilde{L}_1;\cdot)$ and $K_3(\widetilde{L}_2;\cdot)$ vanish identically on the interval $[0,x_{n-3,n}]$. Hence, in view of (3.1),

$$K_3(Q;t)=K_3(\widetilde{Q};t)=n^{-3}\Big[\frac{\sqrt{3}}{216}-\widetilde{B}_3(n\,t)\Big]\geq 0\,,\qquad t\in[x_{3,n},x_{n-3,n}]\,,\tag{3.9}$$

therefore we have to verify condition $K_3(Q;t)\geq 0$ only on the intervals $[0,x_{3,n}]$ and $[x_{n-3,n},1]$. Assuming that this condition is satisfied, for the error constant of Q we have

$$c_3(Q)=\int_0^{x_{3,n}}K_3(Q;t)\,dt+\int_{x_{n-3,n}}^{1}K_3(Q;t)\,dt+\frac{\sqrt{3}(n-6)}{216n^4}\,,\tag{3.10}$$

where the last summand comes from the integral of $K_3(Q;\cdot)$ over the interval $[x_{3,n},x_{n-3,n}]$, and we have used that $\widetilde{B}_3$ has mean value zero on the period.

We aim to minimize $c_3(Q)$, i.e., to minimize the integrals in (3.10) with respect to parameters θ and ϱ, respectively, subject to the requirement $K_3(Q;t)\geq 0$ on the intervals $[0,x_{3,n}]$ and $[x_{n-3,n},1]$.

3.1. POSITIVITY OF $K_3(Q;t)$ ON $[0,x_{3,n}]$

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

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

Thus, we have the equivalence

$$K_3(Q;t)\geq 0,\quad t\in[0,x_{3,n}]\quad\Leftrightarrow\quad\varphi(u)\leq 0,\quad u\in[0,3].\tag{3.11}$$

Before verifying what values of θ ensure condition $\varphi(u) \le 0, u \in [0,3]$, we evaluate the first integral in (3.10):

$$\int_0^{x_{3,n}} K_3(Q;t)\,dt = -\frac{1}{6n^4}\int_0^3 \varphi(u)\,du = \frac{33+\sqrt{3}-\theta}{216n^4}\,. \tag{3.12}$$

To minimize the latter integral and thereby, in view of (3.10), $c_3(Q)$, we have to find the largest value of θ ensuring that $\varphi(u) \le 0,\ u \in [0,3]$.

Case 1: $u \in [0,1]$. In this case

$$\varphi(u) = \frac{u^2}{72}(72u - 108 + \theta),$$

and condition $\varphi(u) \le 0,\ u \in [0,1]$ is equivalent to $\theta \le 36$.

Case 2: $u \in [1,2]$. We set $v = u-1,\ v \in [0,1]$, and using Wolfram's *Mathematica*, find

$$\begin{aligned}\varphi(u) &= u^3 - \frac{108-\theta}{72}\,u^2 - \frac{171+\sqrt{3}+3\theta}{72}\,(u-1)^2\\ &= v^3 - \frac{63+\sqrt{3}}{72}\,v^2 - \frac{1}{2} + \frac{\theta}{36}\Big(-v^2+v-\frac{1}{2}\Big) =: \varphi_1(v)\,.\end{aligned}$$

Since $-v^2+v-1/2<0$ for all $v \in [0,1]$, it follows that $\varphi(u)<0$ for every $u \in [1,2]$ provided θ is big enough; in addition, if the latter condition holds for some θ_0, it will hold also for all $\theta > \theta_0$. The largest value of θ such that $\varphi_1(v) \le 0$ for all $v \in [0,1]$ should be such that φ_1 has a double zero in $(0,1)$, i.e. θ is a zero of $D(\varphi_1)$, the discriminant of φ_1. Using Wolfram's *Mathematica*, we find $D(\varphi_1)$, which is a quintic polynomial of θ with four distinct real zeros: $\theta_1 = -57.5774$, $\theta_2 = 28.0556$, $\theta_3 = 30.7503$ and $\theta_4 = 92.4621$. Only for $\theta = \theta_2$ the polynomial φ_1 has a double zero in $(0,1)$. Therefore, in this case we have the restriction $\theta \le \theta_2 = 28.0556$.

Case 3: $u \in [2,3]$. We set $v = u-2,\ v \in [0,1]$, and find with *Mathematica*

$$\begin{aligned}\varphi(u) &= u^3 - \frac{108-\theta}{72}\,u^2 - \frac{171+\sqrt{3}+3\theta}{72}\,(u-1)^2 - \frac{288-2\sqrt{3}-3\theta}{72}\,(u-2)^2\\ &= \frac{1}{72}\big[72v^3 - (135-\sqrt{3})\,v^2 + (90-2\sqrt{3})\,v - 27 - \sqrt{3} + \theta(v-1)^2\big]\\ &=: \varphi_2(v) = \varphi_2(\theta;v)\,.\end{aligned}$$

Since $\varphi_2(1) = -\sqrt{3}/36 < 0$, it is clear that $\varphi_2(v) < 0$ for all $v \in [0,1]$ provided θ is small enough; moreover, if the above condition on φ_2 is satisfied for some θ_0, then it is satisfied for all $\theta < \theta_0$. The critical value θ^* should be such that φ_2 has a double zero in $(0,1)$, i.e., θ^* is a zero of $D(\varphi_2)$, the discriminant of φ_2. With the help of *Mathematica*, we find

$$\frac{D(\varphi_2)}{8} = \sqrt{3}\,\theta^3 + (171+243\sqrt{3})\theta^2 + (27702+8352\sqrt{3})\theta - 802134 - 386370\sqrt{3}\,.$$

By Descartes' rule of signs, the latter polynomial has a unique positive root θ^*. In fact, using again *Mathematica*, we find that $\theta^* = 27-\sqrt{3} = 25.2679\ldots$ and

$$D(\varphi_2) = 8(\theta-\theta^*)\big[\sqrt{3}\theta^2 + 6(28+45\sqrt{3})\theta + 6(5238+2579\sqrt{3})\big]\,.$$

Thus, the optimal value of θ in *Case 3* is $\theta=\theta^*=27-\sqrt{3}$. Just for one more check, we verify that

$$\varphi_2(\theta^*;v) = v^3 - \frac{3}{2}\,v^2 + \frac{1}{2}\,v - \frac{\sqrt{3}}{36} = \Big(v - \frac{3+2\sqrt{3}}{6}\Big)\Big(v-\frac{3-\sqrt{3}}{6}\Big)^2 \le 0, \qquad v\in[0,1].$$

Summarizing the three cases considered above, we see that the optimal value of θ ensuring that $\varphi(\theta;u)\le 0$ for all $u\in[0,3]$ is $\theta=\theta^*=27-\sqrt{3}$. We have

$$\varphi(\theta^*;u) = u^3 - \frac{81+\sqrt{3}}{72}\,u^2 - \frac{126-\sqrt{3}}{36}\,(u-1)_+^2 - \frac{207+\sqrt{3}}{72}\,(u-2)_+^2\,.$$

The graph of $-\varphi(\theta^*;u)$ is depicted in Figure 1.

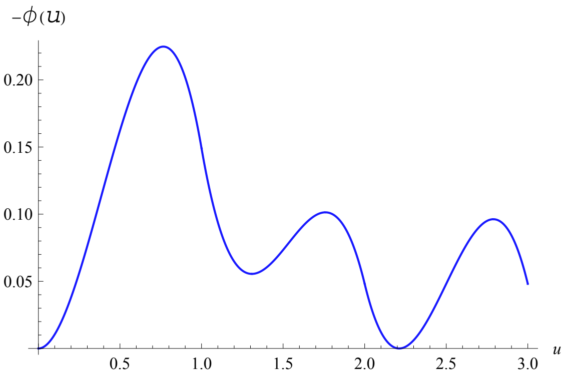

Figure. 1. The graph of $-\varphi(\theta^*;u)$, $0\le u\le 3$.

In view of (3.11), $\theta=\theta^*$ ensures that $K_3(Q;t)\ge 0$ for all $t\in[0,x_{3,n}]$.

With the optimal value $\theta=\theta^*$, the coefficients $\{A_{k,n}\}_0^3$ of quadrature formula (3.7) are given by

$$A_{0,n} = \frac{81+\sqrt{3}}{216n}, \quad A_{1,n} = \frac{126-\sqrt{3}}{108n}, \quad A_{2,n} = \frac{207+\sqrt{3}}{216n}, \quad A_{3,n} = \frac{1}{n}\,,$$

i.e., $\{A_{k,n}\}_0^3$ coincide with the coefficients of quadrature formula Q_n in Theorem 1. Moreover, (3.12) with $\theta = \theta^*$ yields

$$\int_0^{x_{3,n}} K_3(Q;t)\,dt = \frac{3+\sqrt{3}}{108n^4}\,. \tag{3.13}$$

3.2. POSITIVITY OF $K_3(Q;t)$ ON $[x_{n-3,n}, 1]$

We apply (2.1) with $r = 3$ and Q being quadrature formula (3.7) to obtain:

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

Hence,

$$\int_{x_{n-3,n}}^{1} K_3(Q;t)\,dt = \int_0^{x_{3,n}} \widetilde{K}_3(Q;x)\,dx \overset{x=u/n}{=} \frac{1}{n^4}\int_0^3 \psi(\varrho;u)\,du\,,$$

with $\psi(u) = \psi(\varrho;u)$ given by

$$\psi(u) = u^3 - \frac{108-\varrho}{72}\,u^2 - \frac{171-\sqrt{3}+3\varrho}{72}\,(u-1)_+^2 - \frac{288+2\sqrt{3}-3\varrho}{72}\,(u-2)_+^2\,.$$

Now we have the equivalence

$$K_3(Q;t) \ge 0, \quad t \in [x_{n-3,n}, 1] \quad \Leftrightarrow \quad \psi(\varrho;u) \ge 0, \quad u \in [0,3]\,.$$

By a straightforward calculation we obtain

$$\int_{x_{n-3,n}}^{1} K_3(Q;t)\,dt = \frac{\varrho+\sqrt{3}-33}{216n^4}\,, \tag{3.14}$$

therefore, to minimize the error constant $c_3(Q)$, we need to find the smallest ϱ such that $\psi(\varrho;u) \ge 0$ for all $u \in [0,3]$. A necessary condition for the latter requirement to hold is $\varrho \ge 108$, since

$$\psi(\varrho;u) = u^2\Big(u + \frac{\varrho-108}{72}\Big), \qquad u \in [0,1]\,.$$

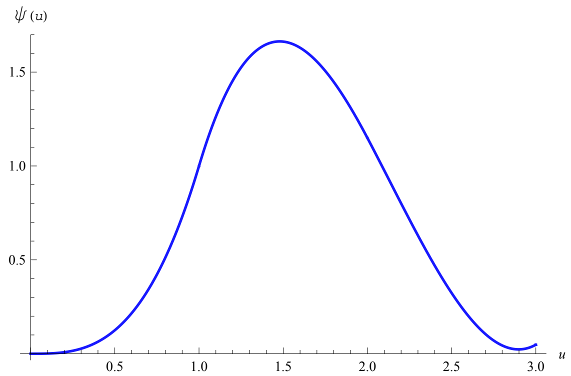

Figure. 2. The graph of $\psi(\varrho^*; u)$, $0 \le u \le 3$.

It turns out that the choice $\varrho = \varrho^* = 108$ is optimal, as it guarantees the non-negativity of ψ on the interval $[0, 3]$, see the graph of $\psi(\varrho^*; \cdot)$ in Figure 2.

With $\varrho = \varrho^*$, coefficients $\{A_{k,n}\}_{k=n-3}^{n}$ of quadrature formula (3.7) are given by

$$A_{n-3,n} = \frac{297 - \sqrt{3}}{216n}, \quad A_{n-2,n} = \frac{\sqrt{3} - 18}{108n}, \quad A_{n-1,n} = \frac{495 - \sqrt{3}}{216n}, \quad A_{n,n} = 0\,.$$

Let us summarize: with the optimal values $(\theta\,, \varrho) = (\theta^*\,, \varrho^*) = (27 - \sqrt{3}, 108)$ the nodes of quadrature formula (3.7) are given in Table 1:

Table 1. The coefficients of quadrature formula (3.7).

$A_{0,n}$	$A_{1,n}$	$A_{2,n}$	$A_{k,n},\ 3 \le k \le n-1$
$\frac{81+\sqrt{3}}{216n}$	$\frac{126-\sqrt{3}}{108n}$	$\frac{207+\sqrt{3}}{216n}$	$\frac{1}{n}$
$A_{n-3,n}$	$A_{n-2,n}$	$A_{n-1,n}$	$A_{n,n}$
$\frac{297-\sqrt{3}}{216n}$	$\frac{\sqrt{3}-18}{108n}$	$\frac{495-\sqrt{3}}{216n}$	0

It is clear now that (3.7) is the positive definite quadrature formula Q_n in Theorem 1.

From (3.14) with $\varrho = \varrho^*$ we find

$$\int_{x_{n-3,n}}^{1} K_3(Q; t)\, dt = \frac{75 + \sqrt{3}}{216 n^4}\,. \tag{3.15}$$

Now (3.10), (3.13) and (3.15) yields

$$c_3(Q_n) = \frac{3+\sqrt{3}}{108n^4} + \frac{75+\sqrt{3}}{216n^4} + \frac{\sqrt{3}(n-6)}{216n^4} = \frac{\sqrt{3}}{216n^3} + \frac{27-\sqrt{3}}{72n^4},$$

which proves (1.10).

To prove the last claim of Theorem 1, we apply Proposition 1(ii) with $Q = Q_n$. Since $A_{k,n} = 1/n$ for $3 \le k \le n-4$, we have, with $f_i = f(x_{i,n})$,

$$\big|R[Q_n; f]\big| \le B[Q_n; f] = \Big|\sum_{k=0}^{3} \big(A_{k,n} - A_{n-k,n}\big)\big(f_{n-k} - f_k\big)\Big|. \tag{3.16}$$

On using

$$A_{0,n} - A_{n,n} = \tfrac{81+\sqrt{3}}{216n}, \qquad A_{1,n} - A_{n-1,n} = -\tfrac{243+\sqrt{3}}{216n},$$
$$A_{2,n} - A_{n-2,n} = \tfrac{243-\sqrt{3}}{216n}, \qquad A_{3,n} - A_{n-3,n} = -\tfrac{81-\sqrt{3}}{216n}$$

and the explicit form of finite differences,

$$\Delta^m f_i = \sum_{k=0}^{m} (-1)^{m-k} \binom{m}{k} f_{i+k},$$

we obtain from (3.16), after rearrangement,

$$B[Q_n; f] = \frac{1}{216n}\left|81\big(\Delta^3 f_{n-3} - \Delta^3 f_0\big) + \sqrt{3}\big(\Delta^2 f_{n-2} + \Delta^2 f_{n-3} - \Delta^2 f_0 - \Delta^2 f_1\big)\right|.$$

The proof of Theorem 1 is complete. □

Proof of Corollary 1. Since $\widetilde{Q}_n[f] = Q_n[\widetilde{f}]$ and $\widetilde{f}_i = f_{n-i}$, $0 \le i \le n$, we deduce from (3.16) that $B[\widetilde{Q}_n; f] = B[Q_n; f]$, which proves the first claim of Corollary 1. The second claim follows from Proposition 1(iii). □

ACKNOWLEDGEMENT. The authors were supported by the Sofia University Research Fund under Contract 80-10-11/2017. The third author acknowledges the support of the Bulgarian National Research Fund through Contract DN 02/14.

4. REFERENCES

[1] Avdzhieva, A., Nikolov, G.: Asymptotically optimal definite quadrature formulae of 4th order. *J. Comput. Appl. Math.*, **311**, 2017, 565–582.

[2] Braß, H.: *Quadraturverfahren.* Vandenhoeck & Ruprecht, Göttingen, 1977.

[3] Förster, K.-J.: Survey on stopping rules in quadrature based on Peano kernel methods. *Suppl. Rend. Circ. Math. Palermo*, Ser. II **33**, 1993, 311–330.

[4] Jetter, K.: Optimale Quadraturformeln mit semidefiniten Peano-Kernen. *Numer. Math.* **25**, 1976, 239–249.

[5] Köhler, P., Nikolov, G.: Error bounds for optimal definite quadrature formulae. *J. Approx. Theory*, **81**, 1995, 397–405.

[6] Lange, G.: *Beste und optimale definite Quadraturformel*. Ph.D. Thesis, Technical University Clausthal, Germany, 1977.

[7] Lange, G.: Optimale definite Quadraturformel. In: *Numerische Integration* (G. Hämmerlin, ed.), ISNM vol. 45, Birkhäuser, Basel, Boston, Stuttgart, 1979, pp. 187–197.

[8] Nikolov, G.: On certain definite quadrature formulae. *J. Comput. Appl. Math.*, **75**, 1996, 329–343.

[9] Peano, G.: Resto nelle formule di quadratura espresso con un integrale definito. *Atti della Reale Accademia dei Lincei: Rendiconti* (Ser. 5), **22**, 1913, 562–569.

[10] Schmeisser, G.: Optimale Quadraturformeln mit semidefiniten Kernen. *Numer. Math.* **20**, 1972, 32–53.

Received on September 8, 2017

Ana Avdzhieva, Vesselin Gushev, Geno Nikolov

Faculty of Mathematics and Informatics
"St. Kl. Ohridski" University of Sofia
5, J. Bourchier blvd., BG-1164 Sofia
BULGARIA

e-mails: aavdzhieva@fmi.uni-sofia.bg
v_gushev@fmi.uni-sofia.bg
geno@fmi.uni-sofia.bg