Journal of Computational and Applied Mathematics 311 (2017) 565–582

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Asymptotically optimal definite quadrature formulae of 4th order☆

Ana Avdzhieva, Geno Nikolov*

Faculty of Mathematics and Informatics, Sofia University "St. Kliment Ohridski", 5 James Bourchier Blvd., 1164 Sofia, Bulgaria

ARTICLE INFO

Article history:
Received 9 May 2016
Received in revised form 23 August 2016

MSC:
41A55
65D30
65D32

Keywords:
Asymptotically optimal definite quadrature formulae
Peano kernel representation
Euler–Maclaurin type summation formulae
A posteriori error estimates

ABSTRACT

We construct several sequences of asymptotically optimal definite quadrature formulae of fourth order and evaluate their error constants. Besides the asymptotical optimality, an advantage of our quadrature formulae is the explicit form of their weights and nodes. For the remainders of our quadrature formulae monotonicity properties are established when the integrand has a non-negative or non-positive fourth derivative, and a-posteriori error estimates are proven.

1. Introduction

We study quadrature formulae of the form

$$Q_n[f] = \sum_{i=1}^{n} a_{i,n} f(\tau_{i,n}), \quad 0 \le \tau_{1,n} < \tau_{2,n} < \cdots < \tau_{n,n} \le 1 \tag{1}$$

for approximate evaluation of the definite integral

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

Our interest is in definite quadrature formulae. Let us recall some definitions.

Definition 1. Quadrature formula (1) is said to be *definite of order* r, $r \in \mathbb{N}$, if there exists a real non-zero constant $c_r(Q_n)$ such that its remainder functional admits the representation

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

for every $f \in C^r[0, 1]$, with some $\xi \in [0, 1]$ depending on f.

Furthermore, Q_n is called positive definite (resp., negative definite) of order r, if $c_r(Q_n) > 0$ ($c_r(Q_n) < 0$).

☆ This work was supported by the Sofia University Research Fund through Contract no. 30/2016.

* Corresponding author.
E-mail addresses: aavdzhieva@fmi.uni-sofia.bg (A. Avdzhieva), geno@fmi.uni-sofia.bg (G. Nikolov).

http://dx.doi.org/10.1016/j.cam.2016.08.022
0377-0427/

Obviously, if Q_n is a definite quadrature formula of order r, then Q_n has *algebraic degree of precision* $r-1$ (in short, $ADP(Q_n)=r-1$), i.e., $R[Q_n;f]=0$ whenever f is an algebraic polynomial of degree at most $r-1$, and $R[Q_n;x^r]\neq 0$.

Throughout this paper, by r-positive (r-negative) function f we shall mean a function $f\in C^r[0,1]$ such that $f^{(r)}\geq 0$ ($f^{(r)}\leq 0$) on the interval $[0,1]$.

The importance of definite quadrature formulae of order r lies in the one-sided approximation they provide for $I[f]$ when the integrand f is r-positive (r-negative). If, e.g., $\{Q^+,\ Q^-\}$ is a pair of a positive and a negative definite quadrature formula of order r and f is r-positive, 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 automatic numerical integration algorithms (see [1] for a survey). Most of quadratures used in practice (e.g., quadrature formulae of Gauss, Radau, Lobatto, Newton–Cotes) are definite of certain order.

Definite n-point quadrature formulae with the smallest positive or the largest negative error constant are called optimal definite quadrature formulae. Let us emphasize that throughout this paper by "optimal" we mean a quadrature formula with the smallest possible error constant. Some authors (e.g. [2–5]) call "optimal" quadratures with a maximal (algebraic, trigonometric, spline, etc.) degree of precision, we however give preference for this case to the term "Gauss-type".

Let us set

$$c_{n,r}^+ := \inf\{c_{n,r}(Q_n) : Q_n \text{ is positive definite of order } r\},$$
$$c_{n,r}^- := \sup\{c_{n,r}(Q_n) : Q_n \text{ is negative definite of order } r\}.$$

It should be pointed out that it is fairly not obvious that the above infimums are attained or that the optimal definite quadrature formulae are unique. The existence of optimal definite quadrature formulae was first proven by Schmeisser [6] for even r, and for arbitrary r and more general boundary conditions by Jetter [7] and Lange [8]. The uniqueness has been proven by Lange [8,9]. For even r, Lange [8] has shown that

$$\begin{aligned} c_{n,r}^+ &= -\frac{B_r(j/2)}{n^r}\Big(1+O(n^{-1})\Big) \quad \text{if } r=4m+2j,\\ c_{n,r}^- &= -\frac{B_r(j/2)}{n^r}\Big(1+O(n^{-1})\Big) \quad \text{if } r=4m+2-2j \end{aligned} \tag{2}$$

for $j=1,2$, where B_r is the rth Bernoulli polynomial with leading coefficient $1/r!$. Schmeisser [6] proved that the same result holds for optimal definite quadrature formulae with equidistant nodes.

The n-point optimal positive definite and the $(n+1)$-point optimal negative definite quadrature formulae of order 2 are well-known: these are the nth compound midpoint and trapezium quadrature formulae, respectively. The case $r=2$ is exceptional, as for $r\geq 3$ the optimal definite quadrature formulae are not known. For $3\leq n\leq 30$, the n-point optimal definite quadrature formulae of order 3 and the n-point optimal positive definite quadrature formulae of order 4 have been computed numerically by Lange [8].

It is a general observation about the optimality concept in quadratures that, even though the existence and the uniqueness of the optimal quadrature formulae (for instance, in the non-periodic Sobolev classes of functions) is established, the optimal quadrature formulae remain unknown. This fact severely reduces the practical importance of optimal quadratures. The way out of this situation is to look for quadrature formulae which are nearly optimal, e.g., for sequences of asymptotically optimal quadrature formulae.

Definition 2. Let $\{Q_n\}_{n=n_0}^{\infty}$ be a sequence of positive (resp, negative) definite quadrature formulae of order r. Q_n is said to be *asymptotically optimal* positive (negative) definite quadrature formula of order r, if

$$\lim_{n\to\infty}\frac{c_r(Q_n)}{c_{n,r}^+}=1 \quad \text{resp.,} \qquad \lim_{n\to\infty}\frac{c_r(Q_n)}{c_{n,r}^-}=1.$$

In [6] Schmeisser proposed an approach for construction of asymptotically optimal definite quadrature formulae of even order r with equidistant nodes. Köhler and Nikolov [10] have studied Gauss-type quadrature formulae associated with spaces of splines with double and equidistant knots, and as a result obtained bounds for the best constants $c_{n,r}^+$ and $c_{n,r}^-$. In particular, it has been shown in [10] that for even r the corresponding Gauss-type quadrature formulae are asymptotically optimal definite quadrature formulae. Motivated by this result, in [11] Nikolov found explicit recurrence formulae for the evaluation of the nodes and the weights of the Gaussian formulae for the spaces of cubic splines with double equidistant knots, and proposed a numerical procedure for the construction of the Lobatto quadrature formulae for the same spaces of splines. According to [10], the Gauss and the Lobatto quadrature formulae for these spaces of splines are respectively asymptotically optimal positive definite and asymptotically optimal negative definite, of order 4.

Although the evaluation of Gauss-type quadrature formulae for spaces of splines (also with single knots, because of their asymptotical optimality in certain Sobolev classes, see [12]) is highly desirable, there is a serious problem occurring already with the splines of degree 3, and its difficulty increases with the splines degree: the mutual displacement of the nodes of the quadratures and the splines knots is unknown. For justifying the location of the quadrature abscissae with respect to the knots of the space of splines, additional assumptions are to be made. For instance, in a recent paper [2] Ait-Haddou, Bartoň