Definite quadrature formulae of order 3 with equidistant nodes

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We study quadrature formulae of the form

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

for approximate evaluation of the definite integral

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

Our interest is in definite quadrature formulae.

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 $c_r(Q)$ such that its remainder functional admits the representation

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

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

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 ointegration interval $[0,1]$.

Definition 2.
A function $f \in C^r[0,1]$ is called r-positive (r-negative) if $f^{(r)}(x) \geq 0$ (resp. $f^{(r)}(x) \leq 0$) for every $x \in [0,1]$.

Introduction

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 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.

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. They are respectively positive and negative definite of order 2. Moreover, Q_n^{Mi} and Q_{n+1}^{Tr} are the optimal definite quadrature formulae of order 2. 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 quadratura formula of order 2, and $c_2(Q_{n+1}^{Tr}) = -\frac{1}{12n^2}$ is the largest error constant among all $(n+1)$-point negative definite quadrature formulae of second order.

Introduction

The optimal definite quadrature formulae of higher order are not known explicity, although their existance and uniqueness is known. Schmeisser constructed optimal definite quadrature formulae of even order with equidistant knots. Köhler and Nikolov showed that certain Gauss-type quadratures for spaces of polynomials with double equidistant knots are asymptotically optimal definite quadrature formulae, and based on this result, Nikolov proposed an algorithm for the construction of asymptotically optimal definite quadrature formulae of order 4. In a recent paper Nikolov and Avdzhieva constructed sequences of asymptotically optimal definite quadrature formulae of order 4 and moreover, for suitable pairs of such definite quadratures 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 rectangles rules,

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

If f is an 1-positive (nondecreasing) function, then $R[Q_+; f] \geq 0$, $R[Q_-; f] \leq 0$. We have

$$|R[Q_\pm; f]| \leq Q_-[f] - Q_+[f] = \frac{1}{n}(f(1) - f(0)),$$

and these inequalities illustrate an a-posteriori error estimates without using the derivatives of the function.

Introduction

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) is called:

- *symmetrical*, if

$$a_k = a_{n-k}\,, \qquad k = 0, \ldots, n\,; \tag{2}$$
$$x_k = 1 - x_{n-k}\,, \qquad k = 0, \ldots, n\,; \tag{3}$$

- *nodes-symmetrical*, if only condition (3) is satisfied;
- Quadrature formula

$$\widetilde{Q}[f] = \widetilde{Q}[Q; f] := \sum_{k=0}^{n} a_k\, f(x_{n-k}) \tag{4}$$

is called the *reflected quadrature formula* to (1).

Thus, 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.

Notations

For $n \in \mathbb{N}$ we set

$$x_{k,n} = \frac{k}{n}, \quad k = 0, \ldots, n; \qquad y_{\ell,n} = \frac{2\ell - 1}{2n}, \quad \ell = 1, \ldots, n\,.$$

The compound trapezium and midpoint quadrature formulae are denoted by Q_{n+1}^{Tr} and Q_n^{Mi}, respectively, i.e.,

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

$$Q_n^{Mi}[f] = \frac{1}{n}\sum_{k=1}^{n} f(y_{k,n})\,.$$

Peano Kernels

If $f \in W_1^r[0,1]$, then for the remainder of the quadrature formula Q stands

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

where $K_r(Q;t)$ is r-th Peano kernel of Q.

Peano Kernels

An explicit representations of $K_r(Q_n; t)$ for $t \in [0, 1]$ are:

$$K_r(Q;t) = \frac{(1-t)^r}{r!} - \frac{1}{(r-1)!} \sum_{i=0}^{n} a_i (x_i - t)_+^{r-1}, \qquad (5)$$

$$K_r(Q;t) = (-1)^r \left[\frac{t^r}{r!} - \frac{1}{(r-1)!} \sum_{i=0}^{n} a_i (t - x_i)_+^{r-1} \right]. \qquad (6)$$

Definite Quadrature Formulae of Order 3

Our interest is in definite quadrature formulae in Sobolev class $W_1^3[0,1]$.
Unlike the definite quadrature formulae of even order, definite quadratures of odd order are never symmetric. Somewhat unexpectedly, this phenomenon turns out to be an advantage rather than disadvantage. For instance, when reflecting the nodes of a positive definite quadrature formula of odd order (keeping the weights unchanged), we obtain a negative definite quadrature formula and vice versa.

Definite Quadrature Formulae of Order 3

We construct sequences of definite quadrature formulae of order 3 based on equidistant nodes, i.e., they use the nodes of either the rectangles or the trapezium quadrature formulae and, excluding the coefficients of the boundary three or four nodes, have the same coefficients. A kind of optimization is performed for the choice of the boundary coefficients so that the error constants of constructed quadratures are as small in absolute value as possible.

Assume that $f \in W_1^3$. Then

$$I[f] = Q_{n+1}^{Tr}[f] - \frac{1}{12n^2}\left[f'(1) - f'(0)\right] - \frac{1}{n^3}\int_0^1 \widetilde{B}_3(nx) f'''(x)\, dx\,, \quad (7)$$

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

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

The Approach

We rewrite formula (7) in the following form:

$$
\begin{aligned}
I[f] =& Q_{n+1}^{Tr}[f] - \frac{1}{12\,n^2}\left[f'(1) - f'(0)\right] - \frac{\sqrt{3}}{216\,n^3}\left[f''(1) - f''(0)\right] \\
&+ \frac{1}{n^3}\int_0^1 \left(\frac{\sqrt{3}}{216} - \widetilde{B}_3(nx)\right) f^{(3)}(x)\,dx \\
=:& \widetilde{Q}[f] + R[\widetilde{Q}; f]\,,
\end{aligned}
\tag{8}
$$

where

$$
\widetilde{Q}[f] = Q_{n+1}^{Tr}[f] + \frac{1}{12n^2}f'(0) + \frac{\sqrt{3}}{216n^3}f''(0) - \frac{1}{12n^2}f'(1) - \frac{\sqrt{3}}{216n^3}f''(1)\,. \tag{9}
$$

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

$$-\frac{\sqrt{3}}{216} \leq \widetilde{B}_3(x) \leq \frac{\sqrt{3}}{216}, \qquad x \in \mathbb{R}. \tag{10}$$

By (8) and (10) it follows that $\widetilde{Q}$ is a positive definite quadrature formula, however, it is not of the desired form as it involves values of the 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 Approach

For the construction of sequences of definite quadratures based on the compound trapezium formula we use two formulae for numerical differentiation of $f'(0)$.

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

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

Then we approximate $f'(0)$ by

$$f'(0) \approx \alpha\, D_{1,1}[f] + (1-\alpha)\, D_{1,2}[f].$$

The Approach

Again we use two formulae for numerical differentiation of $f''(0)$.

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

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

Then we approximate $f'(0)$ by

$$f''(0) \approx \beta\, D_{2,1}[f] + (1-\beta)\, D_{2,2}[f].$$

We do the same for the approximation of $f'(1)$ and $f''(1)$.

$$f'(1) \approx D^*_{1,1}[f] = \frac{n}{2}\Big[3f(x_{n,n}) - 4f(x_{n-1,n}) + f(x_{n-2,n})\Big],$$

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

$$f''(1) \approx D^*_{2,1}[f] = n^2\,[f(x_{n,n}) - 2f(x_{n-1,n}) + f(x_{n-2,n})],$$

$$f''(1) \approx D^*_{2,2}[f] = n^2\,[f(x_{n-1,n}) - 2f(x_{n-2,n}) + f(x_{n-3,n})].$$

Then we approximate $f'(1)$ and $f''(1)$:

$$f'(1) \approx \gamma\, D^*_{1,1}[f] + (1-\gamma)\, D^*_{1,2}[f],$$

$$f''(0) \approx \delta\, D^*_{2,1}[f] + (1-\delta)\, D^*_{2,2}[f].$$

Next...

We obtain quadrature formulae with coefficients $A_{k,n}$ depending of parameters α, β for $k = 0, 1, 2, 3$ and $A_{k,n}$ depending of parameters γ and δ for $k = n-3, n-2, n-1, n$. After analyzing the quadrature formulae we obtain a family of definite quadrature formulae of order 3 for certain values of parameters α, β, γ and δ . We examine the sequences of definite quadratures to optimize the error constants of constructed quadratures in absolute values.

Results

The positive definite quadrature formulae of order 3 based on Q_{n+1}^{Tr} (optimized by the error constant) is

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

with weights

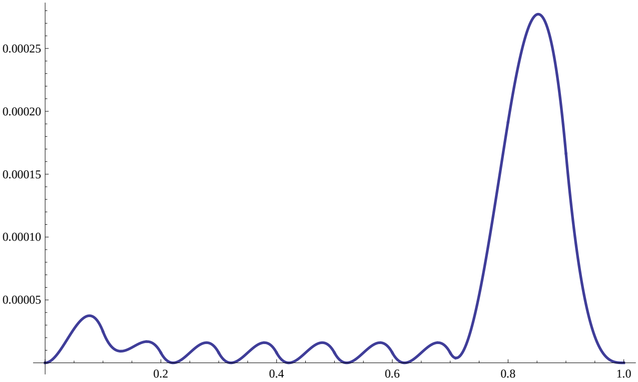
$$A_{0,n} = \frac{81+\sqrt{3}}{216n}, \qquad A_{1,n} = \frac{126-\sqrt{3}}{108n},$$
$$A_{2,n} = \frac{207+\sqrt{3}}{216n}, \qquad A_{k,n} = \frac{1}{n}, \quad 3 \le k \le n-4,$$
$$A_{n-3,n} = \frac{297-\sqrt{3}}{216n}, \qquad A_{n-2,n} = \frac{\sqrt{3}-18}{108n},$$
$$A_{n-1,n} = \frac{495-\sqrt{3}}{216n}, \qquad A_{n,n} = 0.$$

Results

The error constant of $Q_n[f]$ is

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

The Graphics of Peano Kernel $K_3(Q_n[f]; t)$ for $n = 10$



If we have positive definite quadrature formula of order 3, then we can easily construct negative quadrature formula of third order by reflection.
Indeed, let $Q[f]$ is a positive definite quadrature formula of order 3, then the reflected quadrature formula is

$$\widetilde{Q}[f] := Q[\widetilde{f}], \qquad \widetilde{f}(x) = f(1-x).$$

We have $I[f] = I[\widetilde{f}]$ and

$$R[\widetilde{Q}; f] = I[f] - \widetilde{Q}[f] = I[\widetilde{f}] - Q[\widetilde{f}] =$$
$$R[Q; \widetilde{f}] = c_3(Q)\widetilde{f}^{(3)}(\xi) = -c_3(Q)f^{(3)}(\eta),$$

where $\eta = 1 - \xi$, which proves that the reflected quadrature formula is a negative definite quadrature formula of order 3 with the same constant error in absolute value.

A-posteriori Error Estimates of Definite Quadrature Formulae of Order 3

We assume that $f^{(3)} \geq 0$ in $[0, 1]$. Let $Q^+[f] = \sum_{k=0}^{n} A_k\, f(x_k)$ is the constructed positive definite quadrature formula of order 3. Then we obtain the corresponding negative definite quadrature formula of order 3 by reflection

$$Q^-[f] = \sum_{k=0}^{n} A_{n-k}\, f(x_k).$$

We have $R[Q^+; f] \geq 0$ and $R[Q^-; f] \leq 0$. Then

$$0 \leq R[Q^+; f] - R[Q^-; f] = Q^-(f) - Q^+(f)$$

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,

$$c_r(\widetilde{Q}) = -c_r(Q)\,. \tag{11}$$

(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

$$\left|R[Q^*;f]\right| \le B[Q;f] := \left|\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \left(a_k - a_{n-k}\right)\left(f(x_{n-k}) - f(x_k)\right)\right|. \tag{12}$$

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

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

with coefficients

$$\begin{aligned}
A_{0,n} &= \tfrac{81+\sqrt{3}}{216n}, & A_{1,n} &= \tfrac{126-\sqrt{3}}{108n}, \\
A_{2,n} &= \tfrac{207+\sqrt{3}}{216n}, & A_{k,n} &= \tfrac{1}{n}, \quad 3 \leq k \leq n-4, \\
A_{n-3,n} &= \tfrac{297-\sqrt{3}}{216n}, & A_{n-2,n} &= \tfrac{\sqrt{3}-18}{108n}, \\
A_{n-1,n} &= \tfrac{495-\sqrt{3}}{216n}, & A_{n,n} &= 0.
\end{aligned}$$

is positive definite of order 3 with the error constant

$$c_3(Q_n) = \frac{\sqrt{3}}{216n^3} + \frac{27-\sqrt{3}}{72n^4}. \qquad (13)$$

Summary of the Results

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

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

where

$$f_i = f(x_i)\,, \qquad i = 0\,\ldots,n\,,$$

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

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

Summary of the Results

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

Corollary 1.

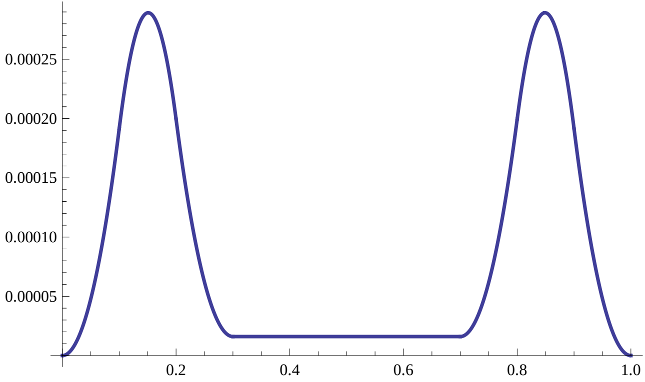
The reflected to Q_n quadrature formula $\widetilde{Q}_n$ is negative definite of order 3 with the error constant $c_3(\widetilde{Q}_n) = -c_3(Q_n)$.

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

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

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

The Graphics of Peano Kernel $K_3(Q_n^-[f] - Q_n^+[f]; t)$ for $n = 10$



Thank you very much for the attention!