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ON THE EXTREMAL PROPERTIES OF OPEN COMPOSITE TRAPEZOIDAL FORMULAE *1)

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Abstract

It is found that the open composite trapezoidal formulae are the best quadrature formulae under three different senses.

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1. Introduction

Recently, Guessab and Schmeisser, under various different conditions, discussed the "sharp" estimates of the remainder $E(f;x_1)$ for two-symmetric-nodes trapezoidal quadrature formulae with a variable node $x_1 \in [a, \frac{1}{2}(a+b)]$,

$$\int_a^b f(t)\mathrm{d}t = \frac{1}{2}(f(x_1)+f(a+b-x_1))(b-a)+E(f;x_1).$$

Actually, there are many differences among the real meanings of all these so called "sharp" estimates, but they are not distinguished in [1] and thus do not lead to further results[2]. More importantly, restrictions on the numbers and symmetry of nodes of the quadrature formula family make the applications of these formulae greatly inconvenient. Imagine that if in a practical situation the nodes are fixed and hence cannot be chosen freely then we cannot make do on using the above formulae. And even if the nodes may be chosen freely, using the composite version of the above formulae will lead to unnecessary increase of numbers of computing functional values of the integrand. It is not worth doing that in view of computational complexity.

Taking the above reasons into account, we will discuss in this paper the following open composite trapezoidal formulae

$$\int_a^b f(t)\mathrm{d}t \approx Q_{\mathbf{x},\mathrm{OCT}}(f) := f(x_1)(x_1-a)+\sum_{i=1}^{n-1}\frac{f(x_i)+f(x_{i+1})}{2}(x_{i+1}-x_i)+f(x_n)(b-x_n)$$

for the general set of nodes $\mathbf{x}=(x_1,x_2,\cdots,x_n)$,

$$a \le x_1 < x_2 < \cdots < x_n \le b.$$

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It goes without saying that the " open " formulae we call here include the "closed" formulae as their special cases of the extreme case allowing $x_1 = a,\ x_n = b$. Obviously, two- symmetric-nodes trapezoidal formulae are only the simplest special cases of the open composite trapezoidal formulae when $\mathbf{x} = (x_1, a+b-x_1)$. Firstly, we must distinguish the definite meanings of various "sharp" estimates. Under the explanation with the definite meaning, the "sharp" estimate should be properly called " exact" estimate. For example, in 1938, Iyengar[3] proved the following inequality when $|f'(t)| \le K$

$$\Big| \int_a^b f(t)\mathrm{d}t - \frac{f(a)+f(b)}{2}(b-a) \Big| \le \frac{K}{4}(b-a)^2 - \frac{(f(b)-f(a))^2}{4K}.$$

Many researchers believe it is a very "good" inequality (see e.g., [4] Sect. 3.7.24), but where on earth is it good? Various generalizations about it still continue to appear (see e.g., [1, 5-9]). But all of them just formally generalize the inequality since a clear understanding of the very essential of the trapezoidal rule indicated by it is not achieved.

In this paper we will consider the exact estimates of the remainder of the open composite trapezoidal formulae $Q_{\mathbf{x},\mathrm{OCT}}(f)$ under three different conditions. It is a surprise to find that the formulae $Q_{\mathbf{x},\mathrm{OCT}}(f)$ themselves have three different extremal properties. From the results of the Nikolskii[10] type estimate for the Hölder classes, we find that $Q_{\mathbf{x},\mathrm{OCT}}(f)$ are the best quadrature formulae in the sense of Sard[11]. From the results of the exact estimates for the first order and a special second order Sobolev class when the Lagrange information is given, we find that $Q_{\mathbf{x},\mathrm{OCT}}(f)$ are also the best quadrature formulae in the sense of Chebyshev for the above two function classes, respectively, i.e., it is a central algorithm for the integral(see [12] for the central algorithm).

2. Main Results and their Proofs

2.1 The best quadrature formulae for the Hölder classes in the sense of Sard

For $K > 0,\quad 0 < \alpha \le 1$, let $KH^\alpha[a, b]$ be the Hölder classes on the interval [a, b], whose definitions are as follows,

$$KH^\alpha[a,b] = \Big\{ f :\ |f(t') - f(t)| \le K|t'-t|^\alpha, \quad \forall\ t,\ t' \in [a,b] \Big\}.$$

Theorem 2.1. *Let $f \in KH^\alpha[a,b]$. Then*

$$\Big| \int_a^b f(t)\,dt - Q_{\mathbf{x},\mathrm{OCT}}(f) \Big| \le \frac{K}{\alpha+1}(x_1-a)^{\alpha+1} + \frac{2K}{\alpha+1}\sum_{i=1}^{n-1}\Big(\frac{x_{i+1}-x_i}{2}\Big)^{\alpha+1} + \frac{K}{\alpha+1}(b-x_n)^{\alpha+1}.$$

Moreover, the estimate given by the above inequality is exact in the following sense that there exists a function $f_* \in KH^\alpha[a,b]$ such that the following equality holds

$$\Big| \int_a^b f_*(t)\,dt - Q_{\mathbf{x},\mathbf{w}}(f_*) \Big| = \frac{K}{\alpha+1}(x_1-a)^{\alpha+1} + \frac{2K}{\alpha+1}\sum_{i=1}^{n-1}\Big(\frac{x_{i+1}-x_i}{2}\Big)^{\alpha+1} + \frac{K}{\alpha+1}(b-x_n)^{\alpha+1},$$

where $Q_{\mathbf{x},\mathbf{w}}(f)$ are arbitrary linear quadrature formulae based on the set of nodes $\mathbf{x}$, i. e.

$$Q_{\mathbf{x},\mathbf{w}}(f) := \sum_{i=1}^n w_i f(x_i).$$

Proof. We have

$$\begin{aligned}\int_a^b f(t)\mathrm{d}t - Q_{\mathbf{x},\mathrm{OCT}}(f) = & \int_a^{x_1} (f(t) - f(x_1))\mathrm{d}t + \sum_{i=1}^{n-1}\Big\{ \int_{x_i}^{c_i} (f(t)-f(x_i))\mathrm{d}t \\ & + \int_{c_i}^{x_{i+1}} (f(t) - f(x_{i+1}))\mathrm{d}t \Big\} + \int_{x_n}^b (f(t)-f(x_n))\mathrm{d}t,\end{aligned}$$

where $c_i = (x_i + x_{i+1})/2$. So for any $f \in KH^\alpha[a,b]$, we have

$$\begin{aligned}\Big|\int_a^b f(t)\mathrm{d}t - Q_{\mathbf{x},\mathrm{OCT}}(f)\Big| &\le \int_a^{x_1} K(x_1-t)^\alpha \mathrm{d}t + \sum_{i=1}^{n-1}\Big\{\int_{x_i}^{c_i} K(t-x_i)^\alpha \mathrm{d}t \\ &+ \int_{c_i}^{x_{i+1}} K(x_{i+1}-t)^\alpha \mathrm{d}t\Big\} + \int_{x_n}^b K(t-x_n)^\alpha \mathrm{d}t \\ &= \frac{K}{\alpha+1}(x_1-a)^{\alpha+1} + \frac{2K}{\alpha+1}\sum_{i=1}^{n-1}\Big(\frac{x_{i+1}-x_i}{2}\Big)^{\alpha+1} \\ &+ \frac{K}{\alpha+1}(b-x_n)^{\alpha+1}.\end{aligned}$$

On the other hand, let

$$f_*(t) := \begin{cases} K(x_1-t)^\alpha, & a \le t < x_1; \\ K(t-x_i)^\alpha, & x_i \le t < c_i; \\ K(x_{i+1}-t)^\alpha, & c_i \le t < x_{i+1}, \quad i = 1,\ 2,\ \ldots, n-1; \\ K(t-x_n)^\alpha, & x_n \le t \le b. \end{cases}$$

Obviously, $f_* \in KH^\alpha[a,b]$ and the equality in Theorem 2.1 holds for f_*. The proof is completed.

Theorem 2.1 indicates that when the set of nodes $\mathbf{x}$ are fixed the open composite trapezoidal formulae are the best quadrature formulae that minimize the supremum of the approximate degree to the integration of functions in the Hölder classes, i. e., the open composite trapezoidal formulae are the best quadrature formulae for the Hölder classes $KH^\alpha[a,b]$ in the sense of Sard,

$$\min_{\mathbf{w}\in\mathbb{R}^n}\max_{f\in KH^\alpha[a,b]}\Big|\int_a^b f(t)\mathrm{d}t - Q_{\mathbf{x},\mathbf{w}}(f)\Big| = \max_{f\in KH^\alpha[a,b]}\Big|\int_a^b f(t)\mathrm{d}t - Q_{\mathbf{x},\mathrm{OCT}}(f)\Big|.$$

2.2 The best quadrature formulae based on the Lagrange information for the first order Sobolev class

For $K > 0$ and a positive integer r, the Sobolev class $KW^r[a,b]$ on the interval [a, b] is the class of all functions which have absolutely continuous $(r-1)$th derivatives and whose rth derivatives satisfy the following inequality

$$|f^{(r)}(t)| \le K \quad \text{a.e. } t \in [a,b].$$

Note that $KW^1[a,b] \equiv KH^1[a,b]$. Thus, letting $\alpha = 1$ in Theorem 2.1, then for $f \in KW^1[a,b]$ we have

$$\Big|\int_a^b f(t)\mathrm{d}t - Q_{\mathbf{x},\mathrm{OCT}}(f)\Big| \le \frac{K}{2}(x_1-a)^2 + \frac{K}{4}\sum_{i=1}^{n-1}(x_{i+1}-x_i)^2 + \frac{K}{2}(b-x_n)^2.$$

The following theorem indicates that the formula $Q_{\mathbf{x},\mathrm{OCT}}(f)$ is the best quadrature formula based on the Lagrange information for the first order Sobolev class among all possible (linear or nonlinear regardless) quadrature formulae, while [13] once pointed out it is the best quadrature rule among all linear quadrature formulae.

Theorem 2.2. *Let $f \in KW^1[a,b]$. Then*

$$\Big|\int_a^b f(t)\,dt - Q_{\mathbf{x},\mathrm{OCT}}(f)\Big| \le \frac{K}{2}(x_1-a)^2 + \frac{K}{4}\sum_{i=1}^{n-1}\Big\{(x_{i+1}-x_i)^2 - \Big(\frac{f(x_{i+1})-f(x_i)}{K}\Big)^2\Big\} + \frac{K}{2}(b-x_n)^2.$$

Moreover, the estimate given by the inequality is exact in the following sense, i.e., for any $f \in KW^1[a,b]$ there exist u_f and $l_f \in KW^1[a,b]$ such that $u_f(x_i) = l_f(x_i) = f(x_i)$, $i =$

1, 2, …, n, *and the following equality holds*

$$\int_a^b u_f(t)\,dt - Q_{\mathbf{x},\mathrm{OCT}}(f) = Q_{\mathbf{x},\mathrm{OCT}}(f) - \int_a^b l_f(t)\,dt = \frac{K}{2}(x_1-a)^2 + \frac{K}{4}\sum_{i=1}^{n-1}\Big\{(x_{i+1}-x_i)^2 - \Big(\frac{f(x_{i+1})-f(x_i)}{K}\Big)^2\Big\} + \frac{K}{2}(b-x_n)^2.$$

The operator $\mathcal{L}_x(f) : KW^1[a,b] \to \mathrm{R}^n$ defined by

$$\mathcal{L}_x(f) := (f(x_1), f(x_2), \dots, f(x_n))$$

is called the Lagrange information operator on the set of nodes $\mathbf{x}$. Theorem 2.2 suggests that when we are given the Lagrange information $\mathcal{L}_x(f)$ on the set of nodes $\mathbf{x}$ for a function $f \in KW^1[a,b]$, the open composite trapezoidal formulae $Q_{\mathbf{x},\mathrm{OCT}}(f)$ are the best quadrature formulae that minimize the supremum of the integral approximate degree, i. e.,

$$\min_{Q\in\mathrm{R}} \max_{\substack{\bar f \in KW^1[a,b]\\ \mathcal{L}_x(\bar f)=\mathcal{L}_x(f)}} \Big|\int_a^b \bar f(t)\mathrm{d}t - Q\Big| = \max_{\substack{\bar f \in KW^1[a,b]\\ \mathcal{L}_x(\bar f)=\mathcal{L}_x(f)}} \Big|\int_a^b \bar f(t)\mathrm{d}t - Q_{\mathbf{x},\mathrm{OCT}}(f)\Big|.$$

Now we give a result for periodic functions in $KW^1[a,b]$. Let $K\tilde W^1[a,b]$ be the subclass of $KW^1[a,b]$ consisting of all periodic functions with period $b-a$ and

$$\tilde Q_{\mathbf{x},\mathrm{OCT}}(f) = \sum_{i=1}^{n} \frac{f(x_i)+f(x_{i+1})}{2}(x_{i+1}-x_i),$$

where $x_{n+1} := b-a+x_1,\ f(x_{n+1}) := f(x_1)$.

Theorem 2.3. *Let $f \in K\tilde W^1[a,b]$ and $x_n - x_1 < b-a$. Then we have*

$$\Big|\int_a^b f(t)\,dt - \tilde Q_{\mathbf{x},\mathrm{OCT}}(f)\Big| \le \frac{K}{4}\sum_{i=1}^{n}\Big\{(x_{i+1}-x_i)^2 - \Big(\frac{f(x_{i+1})-f(x_i)}{K}\Big)^2\Big\}.$$

Moreover, the estimate given by the inequality is exact in the following sense, i.e., for any $f \in K\tilde W^1[a,b]$ there exist u_f and $l_f \in K\tilde W^1[a,b]$ such that $u_f(x_i) = l_f(x_i) = f(x_i)$, $i =$ 1, 2, …, n, and the above equality holds true.

Proof. Since f is periodic and $x_n - x_1 < b-a$, it can be periodically continued to $[b, x_{n+1}]$. Further, it is obvious that the following equality is valid

$$\int_a^b f(t)\mathrm{d}t = \int_{x_1}^{x_{n+1}} \tilde f(t)\mathrm{d}t,$$

where $\tilde f$ is the periodic continuation of f. For $i = 1, 2, \dots, n$, let

$$u_{\tilde f}(t) := \begin{cases} \tilde f(x_i) + K(t-x_i), & x_i \le t < (x_i+x_{i+1})/2 + (\tilde f(x_{i+1}) - \tilde f(x_i))/(2K); \\ \tilde f(x_{i+1}) + K(x_{i+1}-t), & (x_i+x_{i+1})/2 + (\tilde f(x_{i+1}) - \tilde f(x_i))/(2K) \le t < x_{i+1}, \end{cases}$$

and

$$l_{\tilde f}(t) := \begin{cases} \tilde f(x_i) - K(t-x_i), & x_i \le t < (x_i+x_{i+1})/2 - (\tilde f(x_{i+1}) - \tilde f(x_i))/(2K); \\ \tilde f(x_{i+1}) - K(x_{i+1}-t), & (x_i+x_{i+1})/2 - (\tilde f(x_{i+1}) - \tilde f(x_i))/(2K) \le t < x_{i+1}. \end{cases}$$

Let $u_f,\ l_f$ be their respective periodic continuation over $[a,b]$. It is easily verified that $l_f,\ u_f \in K\tilde W^1[a,b]$ and

$$l_f(t) \le f(t) \le u_f(t), \quad \forall\ t \in [a,b];$$
$$l_f(x_i) = \tilde f(x_i) = f(x_i) = u_f(x_i), \quad i = 1,\ 2,\ \dots,\ n.$$

Now, a straightforward calculation on using the following inequality

$$\int_a^b l_f(t)\mathrm{d}t \le \int_a^b f(t)\mathrm{d}t \le \int_a^b u_f(t)\mathrm{d}t$$

yields the conclusion as required. The proof is completed.

2.3 The best quadrature formulae based on the Lagrange information for a special second order Sobolev class

For the given set of nodes $\mathbf{x}$, consider a subclass of the second order Sobolev class. Here the subclass consists of functions whose first derivatives equal to zero at the nodes $\mathbf{x}$, i. e.,

$$KW^2_{\mathbf{x}}[a,b] := \Big\{ f \in KW^2[a,b] : \; f'(x_i) = 0, \quad i = 1,\ 2,\ \ldots, n \Big\}.$$

Theorem 2.4. *Let $f \in KW^2_{\mathbf{x}}[a,b]$. Then*

$$\Big| \int_a^b f(t)\,dt - Q_{\mathbf{x},\mathrm{OCT}}(f) \Big| \le \frac{K}{6}(x_1 - a)^3 + \frac{K}{2}\sum_{i=1}^{n-1} \Big\{ \Big(\frac{x_{i+1} - x_i}{4} \Big)^2 - \Big(\frac{f(x_{i+1}) - f(x_i)}{K(x_{i+1} - x_i)} \Big)^2 \Big\} (x_{i+1} - x_i) + \frac{K}{6}(b - x_n)^3.$$

Moreover, the estimate given by the inequality is exact in the following sense, i.e., for $f \in KW^2_{\mathbf{x}}[a,b]$ there exist u_f and $l_f \in KW^2_{\mathbf{x}}[a,b]$ such that $u_f(x_i) = l_f(x_i) = f(x_i), \quad i = 1,\ 2,\ \ldots,\ n$, and the following equality holds

$$\begin{aligned}\int_a^b u_f(t)\,dt - Q_{\mathbf{x},\mathrm{OCT}}(f) &= Q_{\mathbf{x},\mathrm{OCT}}(f) - \int_a^b l_f(t)\,dt \\ &= \frac{K}{6}(x_1 - a)^3 + \frac{K}{2}\sum_{i=1}^{n-1} \Big\{ \Big(\frac{x_{i+1} - x_i}{4} \Big)^2 - \Big(\frac{f(x_{i+1}) - f(x_i)}{K(x_{i+1} - x_i)} \Big)^2 \Big\} (x_{i+1} - x_i) + \frac{K}{6}(b - x_n)^3.\end{aligned}$$

In order to get Theorem 2.4, we first need the following theorem.

Theorem 2.5[14]**.** *Let $f \in KW^2[a,b]$ and*

$$\int_a^b f(t)\,dt = Q_{\mathbf{x},\mathrm{OCT}}(f) - \frac{1}{2}f'(x_1)(x_1 - a)^2 - \frac{1}{12}\sum_{i=1}^{n-1}(f'(x_{i+1}) - f'(x_i)) \Big(1 + \frac{1}{8}(1 - \alpha_i^2)(1 + 3\beta_i^2)\Big)(x_{i+1} - x_i) + \frac{1}{2}f'(x_n)(b - x_n)^2 + R(f).$$

Then the remainder $R(f)$ satisfies the following inequality,

$$|R(f)| \le \frac{K}{6}(x_1 - a)^3 + \frac{K}{32}\sum_{i=1}^{n-1}(1 - \alpha_i^2)(1 - \beta_i^2)(x_{i+1} - x_i)^3 + \frac{K}{6}(b - x_n)^3,$$

where α_i and β_i can be respectively expressed by the the first divided difference of f' and the third divided difference of f as follows,

$$\alpha_i := \frac{[x_i, x_{i+1}]f'}{K},$$

$$\beta_i := \begin{cases} 2\frac{[x_i, x_i, x_{i+1}, x_{i+1}]f}{1-\alpha_i^2} \cdot \frac{x_{i+1} - x_i}{K}, & \text{for } |\alpha_i| \ne 1; \\ 0, & \text{for } |\alpha_i| = 1. \end{cases}$$

Moreover, the estimate given by the inequality is exact in the following sense, i.e., for $f \in KW^2[a,b]$ there exist u_f and $l_f \in KW^2[a,b]$ such that $u_f(x_i) = l_f(x_i) = f(x_i), \quad u'_f(x_i) = l'_f(x_i) = f'(x_i), \quad i = 1,\ 2,\ \ldots,\ n$, and the following equality holds

$$\begin{aligned}R(u_f) &= R(l_f) \\ &= \frac{K}{6}(x_1 - a)^3 + \frac{K}{32}\sum_{i=1}^{n-1}(1 - \alpha_i^2)(1 - \beta_i^2)(x_{i+1} - x_i)^3 + \frac{K}{6}(b - x_n)^3.\end{aligned}$$

Theorem 2.5 gives the asymptotic expansion of the remainder of the open composite trapezoidal formulae for the class $KW^2[a,b]$. However, as far as the class $KW^2_{\mathbf{x}}[a,b]$ is concerned, the main term of the asymptotic expansion disappears. Thereby, the result of Theorem 2.4 can be obtained.

Theorem 2.4 suggests that for a function $f \in KW^2_{\mathbf{x}}[a,b]$ when the Lagrange information $\mathcal{L}_x(f)$ is given on the set of nodes $\mathbf{x}$, the open composite trapezoidal formulae $Q_{\mathbf{x},\mathrm{OCT}}(f)$ are the best quadrature formulae that minimize the supremum of the integral approximate degree.

Theorem 2.5 suggests that for the general Sobolev class $KW^2[a,b]$ when the information is known on the set of nodes $\mathbf{x}$, the structure of the best quadrature formulae is rather complicated and involves the coefficient K of the class. So it is worth paying attention to the fact that the various extremal properties revealed in this paper concentrate so concisely on the open composite trapezoidal formulae.

3. Comments on the Closed Formulae

A quadrature formula is said to be closed if the end nodes belong to the set of nodes, i.e., $x_1 = a, \quad x_n = b$. The estimates given by the above theorems in this paper appear to be very concise for the closed composite trapezoidal quadrature formulae even without saying.

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