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Exit Criteria for Simpson's Compound Rule*

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Abstract. In many automated numerical algorithms, the calculations are stopped when the difference between two successive approximations is less than a preassigned tolerance. The dependability of this procedure for Simpson's compound rule has been investigated. Classes of functions have been determined for which the above criterion is (a) always valid, and (b) asymptotically valid. A new exit rule is proposed which appears to be less conservative than the standard technique.

1. Introduction. Let f be integrable on $[a, a+h]$, and

$$If = I[a, a+h]f(x) = \int_a^{a+h} f(x)\,dx.$$

Simpson's compound rule, with $2m+1$ points, approximates If by

$$\begin{aligned} S^{(m)}f &= S^{(m)}[a, a+h]f(x) \\ &= \frac{h}{6m}\left[f(a) + 4\sum_{j=1}^{m} f(x_{2j-1}) + 2\sum_{j=1}^{m-1} f(x_{2j}) + f(a+h)\right], \end{aligned} \tag{1}$$

where $x_j = a + jh/2m$. A traditional method of applying Simpson's rule is to evaluate $S^{(1)}f, S^{(2)}f, S^{(4)}f, \cdots$ and accept $S^{(2m)}$ as a sufficiently accurate result when

$$|S^{(m)}f - S^{(2m)}f| < \epsilon, \tag{2}$$

where ϵ is the preassigned tolerance. Adaptive routines use essentially the same method applied to a number of subintervals. Such a procedure may be justified in terms of a stopping inequality.

Definition. The inequality

$$|S^{(m)}f - S^{(2m)}f| \geqq |S^{(2m)}f - If|$$

will be referred to as the stopping inequality. The validity of the stopping inequality is sufficient to insure that the value $S^{(2m)}f$, accepted as the final result by the above exit criterion, will be within the tolerance ϵ.

Clenshaw and Curtis [2] have given an example where (2) is satisfied while the error is much greater than ϵ. On the other hand, Lyness [5], among others, has observed that an exit procedure based on (2) is likely to be too conservative when $f^{(4)}$ is Lipschitz continuous.

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The purpose of this paper is to determine classes of functions for which

(a) the stopping inequality is valid for all m,

(b) the stopping inequality is valid for all m greater than some threshold m_0.

On the basis of the analysis presented here, we will also discuss a modification of the standard exit procedure.

2. Functions with Fourth Derivatives of Constant Sign. In this section, we will show that the stopping inequality is valid for all m if $f^{(4)}$ does not change sign on the interval of integration. We will also show that the inequality is sharp. Before doing this, let us establish several lemmas.

LEMMA 1. *Let $f \in C^{(4)}[a, a + h]$. Then*

$$S^{(m)}f - If = \frac{h^4}{m^4} \int_a^{a+h} g_4\left(\frac{m(x - a)}{h}\right) f^{(4)}(x)\, dx,$$

where

$$4!g_4(x) = \tfrac{1}{3}x^3(2 - 3x), \qquad 0 \leqq x \leqq \tfrac{1}{2},$$

and

$$g_4(x) = g_4(1 - x) = g_4(1 + x) \quad \textit{for all } x.$$

Proof. This result follows from the Euler-Maclaurin sum formula. In particular, it can be obtained by setting $q = 4$ in formula (A.5) of [5] and using the symmetry properties of Bernoulli polynomials [1, p. 804].

LEMMA 2. *Let $f \in C^{(4)}[a, a + h]$ and α be a real number. Then*

$$S^{(m)}f - If - \alpha(S^{(2m)}f - If) = \frac{h^4}{m^4} \int_a^{a+h} G_4\left(\frac{m(x - a)}{h}; \alpha\right) f^{(4)}(x)\, dx,$$

where

$$G_4(x; \alpha) = g_4(x) - \alpha 2^{-4} g_4(2x) \quad \textit{for all } x.$$

Proof. This follows directly from Lemma 1.

LEMMA 3. *The functions g_4 and G_4 have the following properties:*

$g_4(x) \geqq 0$ for all x,

$G_4(x; \alpha) \geqq 0$ for all x when $\alpha \leqq 2$,

$G_4(x; \alpha)$ takes on both signs when $\alpha > 2$.

Proof. The first statement follows directly from the definition of g_4. Note that

$$4!G_4(x; \alpha) = \tfrac{1}{3}x^3[3x(\alpha - 1) + 2 - \alpha], \qquad 0 \leqq x \leqq \tfrac{1}{4}.$$

It follows that G_4 is nonnegative on $[0, \frac{1}{4}]$ when $\alpha \leqq 2$. Now, $g_4(x)$ is increasing and $g_4(2x)$ is decreasing on $[\frac{1}{4}, \frac{1}{2}]$; so G_4 is nonnegative there. Then, G_4 is nonnegative everywhere since it is symmetric about $\frac{1}{2}$ and periodic. Finally, note that $4!\,G_4(\frac{1}{2}; \alpha) = \frac{1}{48}$ and the term $3x(\alpha - 1) + 2 - \alpha$ is negative if $\alpha > 2$ and x is near zero. Thus, G_4 takes on both signs when $\alpha > 2$.

We are now ready to prove several theorems concerning the stopping inequality.

THEOREM 1. *Let $f \in C^{(4)}[a, a + h]$ and assume $f^{(4)}$ does not change sign in $[a, a + h]$. Then, the stopping inequality is valid for all m.*

Proof. First, assume $f^{(4)} \geqq 0$. Replace m by $2m$ in Lemma 1 and apply Lemma 3 to obtain $0 \leqq S^{(2m)} - If$. Then, using Lemmas 2 and 3 with $\alpha = 2$, we have

$$0 \leqq S^{(2m)}f - If \leqq S^{(m)}f - S^{(2m)}f,$$

which implies the stopping inequality. The case where $f^{(4)} \leqq 0$ is similar.

We will now show that the stopping inequality is sharp for the class of functions covered by Theorem 1.

THEOREM 2. *Let $0 < K < 1$ and m be a positive integer. Then there exists a function f such that $f^{(4)}$ has constant sign in $[a, a + h]$ and*

$$|S^{(2m)}f - If| > K\,|S^{(m)}f - S^{(2m)}f|.$$

Proof. Let $\alpha = (1 + K)/K$ in Lemma 2 to obtain the equation

$$K(S^{(m)}f - S^{(2m)}f) - (S^{(2m)}f - If) = \frac{Kh^4}{m^4}\int_a^{a+h} G_4\left(\frac{m(x-a)}{h};\frac{1+K}{K}\right)f^{(4)}(x)\,dx.$$

Since the kernel G_4 is negative on part of the interval $[a, a + h]$, we can choose $f^{(4)} \geqq 0$ so that the right-hand side of the above equation is negative. Hence,

$$K(S^{(m)}f - S^{(2m)}f) < S^{(2m)}f - If.$$

Applying Lemma 3 to Lemma 2 with $\alpha = 1$, we see that the left side of this inequality is nonnegative, and the result follows.

3. Asymptotic Validity of the Stopping Inequality.

When $f^{(4)}$ is not of constant sign, we cannot give a rigorous bound such as that given in Theorem 1. However, we can show that under certain conditions the stopping inequality is asymptotically valid; that is, there exists an integer m_0 such that the stopping inequality is satisfied for all $m \geqq m_0$.

THEOREM 3. *Let $f \in C^{(2q+1)}[a, a + h]$ with $q \geqq 2$. Assume $If^{(2r)} = 0$ for $r = 2, 3, \cdots, q - 1$, but $If^{(2q)} \neq 0$. Then, as $m \to \infty$, the stopping inequality is eventually satisfied.*

Proof. Using formula (A.5) of [5], we see that, as $m \to \infty$,

$$S^{(m)}f - If = c_{2q}\frac{h^{2q}}{m^{2q}}\int_a^{a+h} f^{(2q)}(x)\,dx + O(m^{-2q-1}),$$

where c_{2q} is a nonzero constant. From this, we can write

$$\begin{aligned} S^{(2m)}f - If &= c_{2q}\frac{h^{2q}}{2^{2q}m^{2q}}\int_a^{a+h} f^{(2q)}(x)\,dx + O(m^{-2q-1}), \\ S^{(m)}f - S^{(2m)}f &= \frac{c_{2q}h^{2q}}{m^{2q}}\left(1 - \frac{1}{2^{2q}}\right)\int_a^{a+h} f^{(2q)}(x)\,dx + O(m^{-2q-1}). \end{aligned} \tag{3}$$

Hence,

$$\lim_{m\to\infty}\frac{S^{(2m)}f - If}{S^{(m)}f - S^{(2m)}f} = \frac{1}{2^{2q} - 1}, \tag{4}$$

which implies that the stopping inequality is eventually satisfied.

In the limit, the $S^{(2m)}f$ approximation is roughly 2^{2q} times as accurate as the $S^{(m)}f$ approximation. Usually, $q = 2$ and the exit criterion based on (2) is roughly fifteen times too accurate.

Let us now point out that even for functions in $C^{(\infty)}[a, a+h]$, m may have to be very large before the stopping inequality will be satisfied.

THEOREM 4. *Let k be a positive integer. There exists a function* $f \in C^{(\infty)}[a, a+h]$ *such that the stopping inequality fails for the first k applications of Simpson's rule.*

Proof. Without loss of generality, we can assume the interval $[a, a+h]$ to be $[-1, 1]$. Let

$$f(x) = e^{ax} \sin(2^k \pi x),$$

where $a \neq 0$. Then, $f \in C^{(\infty)}[-1, 1]$ and

$$If = 2^k\pi(1 - e^{2a})/e^a(a^2 + 2^{2k}\pi^2) \neq 0.$$

Clearly, $f(x_i) = 0$ at all points x_i required by $S^{(m)}f$, $m = 1, 2, 4, \cdots, 2^k$. Thus, $S^{(m)}f = 0$ for $m = 1, 2, 4, \cdots, 2^k$, and the stopping inequality fails for the first k approximations.

The stopping inequality is not always asymptotically valid. To see this, let $f \in C^{(2)}[0, 1]$ be defined by

$$f(x) = \tfrac{3}{2}F(x, \tfrac{1}{3}) - F(x, \tfrac{1}{5}),$$

where

$$\begin{aligned} F(x, t) &= 0, & 0 \leqq x \leqq t, \\ &= (x - t)^3, & t < x < 1. \end{aligned}$$

In terms of generalized functions,

$$f^{(4)}(x) = 9\delta(x - \tfrac{1}{3}) - 6\delta(x - \tfrac{1}{5});$$

so Lemma 1 implies that

$$S^{(m)}f - If = \frac{3}{m^4}\left[3g_4\left(\frac{m}{3}\right) - 2g_4\left(\frac{m}{5}\right)\right].$$

Using this equation, one can show that the ratio $(S^{(2m)}f - If)/(S^{(m)}f - S^{(2m)}f)$ is periodic and takes on the value 499/285, whenever m is an odd power of 2. Thus, the stopping inequality fails infinitely often as $m \to \infty$.

4. Modified Exit Procedure. If f satisfies the hypothesis of Theorem 3, then (3) implies that

$$\lim_{m\to\infty} \frac{S^{(m)}f - S^{(2m)}f}{S^{(2m)}f - S^{(4m)}f} = 2^{2q}. \tag{5}$$

If $2^{2q} - 1$ is approximated by 2^{2q} in (4), then (4) and (5) imply that the quantity $(S^{(2m)}f - S^{(4m)}f)^2/(S^{(m)}f - S^{(2m)}f)$ is asymptotically close to $S^{(4m)}f - If$. This leads us to propose the following two-step exit rule:

Accept the approximation $S^{(4m)}f$, if

(a) $(S^{(m)}f - S^{(2m)}f)/(S^{(2m)}f - S^{(4m)}f)$ is close to a power of 2, and

(b) $(S^{(2m)}f - S^{(4m)}f)^2/|S^{(m)}f - S^{(2m)}f| \leqq \epsilon$.

Condition (a) serves as a test to determine whether the $O(m^{-2q-1})$ terms are small enough so that the asymptotic formulas will be good approximations, while (b) requires that an asymptotic estimate of the error not exceed ϵ. Lyness [5] has proposed that the standard exit criterion (2) be replaced by $|S^{(m)}f - S^{(2m)}f| \leqq 15\epsilon$. When $q = 2$, one can see from (5) that condition (b) is similar, since it roughly requires that $|S^{(4m)}f - S^{(2m)}f|$ not exceed 16ϵ.

One evident disadvantage of such an exit procedure is that it cannot be applied before the third approximation. Nevertheless, sample calculations given in [7] indicate that the above procedure seems to be less conservative than the standard rule. It was also observed that the quantity in (a) tended to stray away from a power of two near the point at which round-off error began to dominate the truncation error. This quantity might be useful in determining the point of diminishing returns, as suggested by Lyness [6].

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