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NUMERICAL INTEGRATION WITH ERROR CONTROL*

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Proposed are two interval methods for numerical integration of a sufficiently smooth function over a given finite interval. By means of sequential step halving both methods produce infinite inclusion antitone sequences of intervals, which limits fall in the exact value of the integral. The iteration methods are realized in the computer algebra system Maple V Release 4. Numerical experiments are reported, demonstrating the finite convergence principle as a natural termination criterion of iteration processes in an environment for scientific computations.

1. Introduction. Let f be an integrable function on the interval $[a, b]$. Numerical integration consists in the presentation

$$I \equiv \int_a^b f(x)dx = \sum_{i=1}^{m} A_i f(x_i) + R(f).$$

Usually the error term $R(f)$ is dropped and $\sum_{i=1}^{m} A_i f(x_i)$ is taken as an approximation of the integral, $I \approx \sum_{i=1}^{m} A_i f(x_i)$. In Newton–Cotes closed quadrature formulae, which are considered in the following, the nodes are equally spaced,

$$a = x_0 < x_1 < \cdots < x_m = b, \quad x_i = x_0 + ih, \quad h = \frac{b-a}{m}; \tag{1}$$

the A_i's are chosen so that the truncation error $R(f) = 0$ when $f(x)$ is a polynomial of highest possible degree.

One important question in numerical integration methods is the choice of the step size h. An usual approach is the following: first one integrates f using the nodes (1) and computes an approximation value, say I_m, for I; then a new mesh is constructed by step halving, $h/2$, and a new approximation, say I_{2m}, is obtained. Continuing this process one gets an infinite sequence of approximations to I: $I_m, I_{2m}, I_{4m}, \ldots$. The question now is when to stop with subdivision of the integration interval, that is what is the optimal step size, where the round-off error and the truncation error are minimal.

One approach is the development of adaptive integration rules with good termination criteria [3]. Another approach, proposed in [2], is based on the discrete stochastic arithmetic, which is implemented in the CADNA library and allows to estimate the number of exact significant digits of the computed result using the concept of the computed zero @.0. A third approach consists in constructing algorithms with result verification

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to obtain guaranteed bounds (intervals) for the exact value I of the integral. An idea for such an algorithm is given in [4]: first an interval enclosing the error term $R(f)$ is computed; if it is large, the step size is reduced and an enclosure for $R(f)$ is computed again. This process is repeated until the error interval becomes small enough; then an interval for the integral is computed using the last step width. As we shall see in the following, this approach can cause too many useless iterations without producing an optimal result. In [1], an user prescribed tolerance for the width of the enclosing interval serves as a stopping criterion. But it can happen (and this is demonstrated by many examples in [1]) that the desired accuracy can not be achieved, which leads to program termination with an error message without displaying any result.

In this paper we propose two procedures based on known sequential integration rules – the trapezoidal and the Simpson's rules – for enclosing the exact value I of the integral. Both procedures generate infinite inclusion antitone sequences of intervals, which limits contain I. In the computer realization of these procedures a natural stopping criterion is used, the finite convergence principle [6].

The paper is organized as follows. In Section 2 we present the traditional sequential trapezoidal and Simpson's rules for approximate computation of the integral. In Section 3 the corresponding verification algorithms are proposed. Section 4 reports on some numerical results using the computer algebra system Maple V Release 4.

2. Sequential Integration Rules.

2.1. The sequential trapezoidal rule. Assume that f, f', f'' are continuous on $[a, b]$. Let $[a, b]$ be divided into m subintervals using the nodes (1). The trapezoidal rule for approximate computation of I with step size h (see [5]) is

$$T(f; h) = \frac{h}{2}\left(f(x_0) + 2\sum_{i=1}^{m-1} f(x_i) + f(x_m)\right).$$

There exist points $\xi_i \in [x_{i-1}, x_i]$, $i = 1, 2, \dots, n$, so that the truncation error has the form

$$R_T(f; h) = -\frac{h^3}{12}\sum_{i=1}^{m} f''(\xi_i).$$

Therefore, $I = T(f; h) + R_T(f; h)$ holds true.

For any integer $n \geq 1$ let the interval $[a, b]$ be divided into $2^n = 2m$ subintervals of equal width $h = (b - a)/2^n$. The trapezoidal rules $T(f; h)$ and $T(f; 2h)$ for step sizes h and $2h$ respectively obey the relation $T(f; h) = \dfrac{1}{2}T(f; 2h) + h\displaystyle\sum_{i=1}^{m} f(x_{2i-1})$. Denote

$$T(0) = \frac{h}{2}(f(a) + f(b)); \quad T(n-1) = T(f; 2h), \quad T(n) = T(f; h), \quad n \geq 1.$$

The sequential trapezoidal rule is then defined by

$$T(n) = \frac{1}{2}T(n-1) + h\sum_{i=1}^{m} f(x_{2i-1}), \quad n = 1, 2, \dots$$

2.2. Sequential Simpson's Rule. Let f possesses continuous derivative $f^{(4)}(x)$ on the interval $[a, b]$. Divide $[a, b]$ into $2m$, $m \geq 1$, subintervals using the nodes

(2) $$a = x_0 < x_1 < \ldots < x_{2m} = b, \quad x_i = x_0 + ih, \quad h = \frac{b-a}{2m}.$$

Simpson's rule (Simpson's "one-third" rule) is presented by the formula [5]

$$S(f; h) = \frac{h}{3} \sum_{i=1}^{m} \left(f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i}) \right).$$

The truncation error is

$$R_S(f; h) = -\frac{h^5}{90} \sum_{i=1}^{m} f^{(4)}(\xi_i) \quad \text{for some} \quad \xi_i \in [x_{2(i-1)}, x_{2i}];$$

thus $I = S(f; h) + R_S(f; h)$ is valid.

For any integer $n \geq 1$ let $[a, b]$ be divided into $2^n = 2m$ subintervals of equal width $h = (b-a)/2^n$. Assume that the sequential trapezoidal rule is used to obtain $T(0)$, $T(1)$, $\ldots$ $T(n)$; then Simpson's rule $S(n) = S(f; h)$ for 2^n subintervals is defined by the formula

$$S(n) = \frac{1}{3} \left(4T(n) - T(n-1) \right), \quad n = 1, 2, \ldots.$$

3. Verified Quadrature Formulae. In the traditional numerical analysis the error terms in the quadrature formulae are omitted and an approximation value for the integral is delivered. Here we propose quadrature formulae based on the sequential trapezoidal and Simpson's rules, taking into account the truncation error. This allows to compute guaranteed bounds for the exact value of the integral.

3.1. Interval Sequential Trapezoidal Rule. Assume that f satisfies the conditions from section 2.1. Let the interval $[a, b]$ be divided in subintervals using the nodes (1). For any interval $[x] \subseteq [a, b]$ denote by $F([x])$ and $F''([x])$ inclusion isotone interval extensions of f and f'' respectively [7]. Define

$$\begin{aligned} [T](f; h) &= \frac{h}{2} \left(F([x_0, x_0]) + 2 \sum_{i=1}^{m-1} F([x_i, x_i]) + F([x_m, x_m]) \right), \\ [R_T](f; h) &= -\frac{1}{12} h^3 \sum_{i=1}^{m} F''([x_{i-1}, x_i]). \end{aligned}$$

All operations in the above expressions are meant as interval arithmetic ones.

Using the notation $[T](0) = \frac{1}{2} h(F([a, a]) + F([b, b]))$, $[T](n-1) = [T](f; 2h)$, $[T](n) = [T](f; h)$ and $[R_T](n) = [R_T](f; h)$ we obtain

$$[T](n) = \frac{1}{2}[T](n-1) + h \sum_{i=1}^{m} F([x_{2i-1}, x_{2i-1}]), \quad n = 1, 2, \ldots.$$

The formula

(3) $$[IT](n) = [T](n) + [R_T](n), \quad n = 1, 2, \ldots$$

is called interval sequential trapezoidal rule.

3.2. Interval sequential Simpson's rule. Let f satisfies the assumptions from section 2.2. Let $[a, b]$ be divided in subintervals using the nodes (2). For any interval $[x] \subseteq$

$[a,b]$ denote by $F([x])$ and $F^{(4)}([x])$ inclusion isotone interval extensions of f and $f^{(4)}$ respectively [7]. Define further

$$[S](f;h) = \frac{h}{3}\sum_{i=1}^{m}\left(F([x_{2i-2},x_{2i-2}]) + 4F([x_{2i-1},x_{2i-1}]) + F([x_{2i},x_{2i}])\right),$$
$$[R_S](f;h) = -\frac{h^5}{90}\sum_{i=1}^{m}F^{(4)}([x_{2(i-1)},x_{2i}]).$$

Denote $[S](n) = [S](f;h)$, $[R_S](n) = [R_S](f;h)$; then

$$[S](n) = \frac{1}{3}\left(4[T](n) - [T](n-1)\right).$$

The interval sequential Simpson's rule is presented by the formula

$$[IS](n) = [S](n) + [R_S](n), \quad n = 1,2,\ldots. \tag{4}$$

Proposition. *Formulae* (3) *and* (4) *produce infinite sequences of intervals with the following properties:*

(a) $[IT](1) \supseteq [IT](2) \supseteq [IT](3) \supseteq \ldots$, $[IS](1) \supseteq [IS](2) \supseteq [IS](3) \supseteq \ldots$*;*

(b) $I \in [IT](n)$ *and* $I \in [IS](n)$ *for* $n = 1,2,\ldots$*;*

(c) *If for any interval* $[x] \subseteq [a,b]$*,* $F''([x])$ *and* $F^{(4)}([x])$ *are Lipschitzian with constants* L_1*,* $L_2 > 0$*, which do not depend on* $[x]$*, then* $\lim_{n\to\infty}[IT](n) = I$*,* $\lim_{n\to\infty}[IS](n) = I$ *hold true.*

Proof. (a) and (b) follow from the inclusion isotonicity of the interval extensions F, F'' and $F^{(4)}$ as well as of the interval arithmetic operations [6]–[7].

(c) Inclusion antitone interval sequences are always convergent (see [6]) and

$$\lim_{n\to\infty}[IT](n) = \bigcap_{n=1}^{\infty}[IT](n), \quad I \in \bigcap_{n=1}^{\infty}[IT](n).$$

The width $\omega([R_T](n))$ of the error term satisfies the inequality

$$\omega([R_T](n)) \le \frac{1}{12}L(b-a)^4\frac{1}{2^{3n+1}},$$

thus $\lim_{n\to\infty}\omega([R_T](n)) = 0$ and therefore $\lim_{n\to\infty}[IT](n) = I$ is valid. The convergence of the sequence $\{[IS](n)\}_{n=1}^{\infty}$ to I can be shown in similar way.

4. Numerical Examples. For any iterative interval method, which produces an inclusion antitone sequence of intervals $\{[I](n)\}$, whose end points are represented by mashine (finite precision) numbers, there is a natural stopping criterion: the sequence converges in finite number of steps, i. e. there exists an index l, such that $[I](1) \supseteq [I](2) \supseteq \cdots \supseteq [I](l)$, but $[I](l) \subseteq [I](l+1)$. The latter inclusion means that further iterations are useless; $[I](l)$ is displayed as final result.

The interval sequential integration rules (3) and (4) are implemented in the computer algebra system Maple V Release 4. Thereby the INTPAK package is used for rounded interval arithmetic and interval function evaluations.

Example [2]. $\quad I = \displaystyle\int_{-1}^{1} 20\cos(20\,x)\,(2.7\,x^2 - 3.3\,x + 1.2)dx$

• Interval sequential trapezoidal rule

n	$[IT](n)$	$\omega([R_T](n))$
1	$[-10686.16967, 10797.83047]$	—
2	$[-2031.549996, 2024.450032]$	0.41×10^4
3	$[-436.4998695, 407.7286221]$	0.85×10^3
4	$[-58.45268987, 72.98863358]$	0.13×10^3
5	$[-2.202115428, 16.30683464]$	0.19×10^2
6	$[6.119049106, 8.498941338]$	0.24×10^1
7	$[7.167301653, 7.465154589]$	0.29×10^0
⋮	⋮	⋮
12	$[7.316680128, 7.316695437]$	0.91×10^{-5}
13	$[7.316676502, 7.316699055]$	0.11×10^{-6}

The numerical outputs in the above table satisfy the relations

$$[IT](1) \supset [IT](2) \supset \cdots \supset [IT](12), \quad \text{but} \quad [IT](12) \subset [IT](13).$$

This effect is called finite convergence of sequences in computer (rounded) arithmetic. The interval $[IT](12)$ is taken as final result, enclosing the exact value for the integral; this is the optimal interval with respect to the mashine precision (10 decimal digits in the mantissa). The optimal step size is $h = 1/2^{11}$. One can see that the widths of the error intervals $\omega([IT](n))$ in the last column of the table continue to decrease.

• Interval sequential Simpson's rule

The next table presents the numerical outputs with 15 decimal digits in the mantissa (which corresponds to double precision):

n	$[IS](n)$	$\omega([R_S](n))$
1	$[-314930.836265861, 315042.497067503]$	—
2	$[-19710.0101095144, 19663.3232238210]$	0.39×10^5
3	$[-961.253512599698, 914.163154067078]$	0.19×10^4
4	$[-38.8523436021158, 59.3105184338265]$	0.98×10^2
5	$[5.38149054805527, 9.26091255612297]$	0.39×10^1
6	$[7.25054709104315, 7.38620412384172]$	0.14×10^0
⋮	⋮	⋮
12	$[7.31668774717207, 7.31668774739923]$	0.13×10^{-9}
13	$[7.31668774713102, 7.31668774744147]$	0.40×10^{-11}

Since $[IS](1) \supset [IS](2) \supset \cdots \supset [IS](12)$ and $[IS](12) \subset [IS](13)$ hold true, the interval $[IS](12)$ is displayed as final result although the error terms continue to decrease. The optimal step size is $h = 1/2^{11}$.

For the same example in [2] the CADNA software produces a test for the correctness of the numerical approximation to I, providing 12 significant digits in the output: $I \approx 7.3166877472851$; the latter is enclosed by $[IS](12)$.

REFERENCES

[1] Fr. Blomquist. Verifizierende Numerik mit PASCAL–XSC. BCD–Version. Numerische Anwendungen. Hilfs–Module. Bibliothek I. Saarbrücken, 2000.

[2] F. Jézéquel. Numerical accuracy of converging sequences. Mathematics and Education in Mathematics, Proc. 30th Spring Conf. UBM, 2001, 444–449.

[3] W. Gander, W. Gautschi. Adaptive quadrature – revisited. ETH Zürich, Dept. Informatik, Technical Report #306, 1998, 3–22.

[4] R. Lohner. Praktikum "Einschließung bei Differentialgleichungen". Wissenschaftliches Rechnen mit Ergebnisverifikation, U. Kulisch (Hrsg.), Vieweg & Sohn, Braunschweig, 1989.

[5] J. H. Mathews. Numerical methods for computer science, engineering and mathematics. Prentice-Hall, 1987.

[6] R. Moore. Methods and applications of interval analysis. SIAM, Philadelphia, 1979.

[7] H. Ratschek, J. Rokne. Computer methods for the range of functions. Wiley & Sons, 1984.

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ЧИСЛЕНО ИНТЕГРИРАНЕ С КОНТРОЛ НА ГРЕШКАТА

Нели Димитрова

Предложени са два интервални метода за числено пресмятане на определен интеграл от достатъчно гладка функция. Чрез последователно разполовяване на стъпката на интегриране двата метода произвеждат безкрайни, антитонни по включване редици от интервали, чиито граници съвпадат с точната стойност на интеграла. Методите са реализирани програмно в системата за компютърна алгебра Maple V Release 4. Дадени са резултати от числени експерименти, които демонстрират принципа на крайната сходимост като естествен критерий за спиране на итерационен процес, реализиран в програмна среда за научни изчисления.