MATHEMATICS OF COMPUTATION, VOLUME 29, NUMBER 131
JULY 1975, PAGES 806–809

Adaptive Integration and Improper Integrals*

By Seymour Haber

ABSTRACT. Let R be the class of all functions that are properly Riemann-integrable on $[0, 1]$, and let IR be the class of all functions that are properly Riemann-integrable on $[a, 1]$ for all $a > 0$ and for which

$$\lim_{a \to 0^+} \int_a^1 f(x)\, dx$$

exists and is finite. There are computational schemes that produce a convergent sequence of approximations to the integral of any function in R; the trapezoid rule is one. In this paper, it is shown that there is no computational scheme that uses only evaluations of the integrand, that is similarly effective for IR.

In this paper, I will discuss the convergence of the approximations that are produced by adaptive numerical quadrature methods. An adaptive quadrature method is one which does not use the same sequence of quadrature points (the points at which the integrand is evaluated) for all integrands; after the first integrand evaluation it chooses some or all of the succeeding points in a manner dependent on the integrand values found at the points already used. Such a method may be made "automatic" by incorporating in it a stopping procedure, a procedure for deciding when to stop the calculation and report a final value for the integral. In order to discuss convergence, I will deal, formally, with methods that are not automatic. This distinction is not really important; an automatic method can be thought of as part of a larger nonautomatic method, in which the automatic method's stopping criterion is varied so as to produce more and more accurate approximations to the integral.

The purpose of adaptiveness is the efficient handling of integrands which are quite well-behaved in some part of the interval of integration and are ill-behaved in some other part. Thus, Rice has shown [1] that certain adaptive integration schemes can integrate many functions that have singularities of the $x^{-\alpha}$ type as quickly as they, or the quadrature formulas that they are based on, integrate functions that are quite smooth. This is in contrast to what happens with a nonadaptive scheme such as the trapezoid rule. There the use of very closely spaced points in the neighborhood of the singularity entails the use of equally dense points in the rest of the integration interval, which is a waste of effort. As a result, the trapezoid rule with N points approximates $\int_0^1 x^{-1/2}\, dx$ with an error of the order of magnitude of $N^{-1/2}$. The adaptive schemes discussed by Rice approximate this integral to within $O(N^{-2})$ when using the trapezoid formula as their basic quadrature formula.

Received August 9, 1974.

AMS (MOS) subject classifications (1970). Primary 65D30, 02E99.

Key words and phrases. Integrals, improper integrals, numerical analysis, numerical integration, numerical quadrature, quadrature, singularities, Riemann integral.

*This work was supported in part by a Fulbright-Hays Senior Postdoctoral grant.

Copyright © 1975, American Mathematical Society

License or copyright restrictions may apply to redistribution; see https://www.ams.org/journal-terms-of-use

A natural question is: How general are such schemes? Can one find adaptive quadrature procedures that will handle the full range of integrable singularities? We cannot consider the generality of Lebesgue-integrable functions, where the integral is not determined by the values of the function on any countable set of points; but we may consider improper Riemann integrals. It is well known that many nonadaptive quadrature schemes—the trapezoid rule, Simpson's rule, and the Gauss-Legendre sequence—have the property of converging to the true integral for all *properly* Riemann-integrable functions. Can any adaptive procedure do the same for all improperly-integrable functions? To make clearer the set of functions considered, let us define IR to be the set of all real functions f that are defined on $(0, 1]$, properly Riemann-integrable on $[a, 1]$ for every a in $(0, 1]$, and for which

$$\int_0^1 f(x)\,dx = \lim_{a\to 0^+} \int_a^1 f(x)\,dx$$

exists and is finite. It is known [2] that no nonadaptive linear quadrature scheme converges for all functions in IR. I shall show that no adaptive scheme does, either.

Let me first describe more carefully what an adaptive procedure does: It starts by evaluating the integrand f at a particular point x_1. Thereafter, whenever it has evaluated the integrand, say, the nth time, at some point, x_n, it goes through a finitely long calculation involving the numbers $x_1, x_2, \ldots, x_n$ and $f(x_1), f(x_2), \ldots, f(x_n)$ and, as a result, specifies two things: first, whether or not to report, at this stage of the overall procedure, a number that is an approximation to the integral (and specifies the number itself, if the decision is positive); second, it specifies the next point, x_{n+1}, at which the integrand is to be evaluated. Of course, for some n the decision procedure may be almost vacuous; it may have been decided, after the $n-1$st evaluation, to evaluate the function at a certain set of, say, 10 points before doing any other arithmetic or decision-making, so that after the nth evaluation, the procedure automatically continues to the $n+1$st. Let me emphasize that we are considering only procedures in which the decisions made—whether to report, what to report, the value of x_{n+1}—depend only on the numbers $x_1, \ldots, x_n$ and $f(x_1), \ldots, f(x_n)$. That is, if g were another integrand with $f(x_i) = g(x_i)$, $i = 1, 2, \ldots, n$, exactly the same decisions would be made for g, at that stage, as for f. (One may imagine the possibility of procedures for which this would not be the case, namely ones in which the decisions were based, perhaps, on some kind of analysis of the algorithm for calculating f rather than only on the values found.) We need make no further restrictions on the nature of the decision method, such as recursiveness.

I shall consider only infinite adaptive procedures—those which must report an infinite sequence of approximations to the integral. Denoting the successive approximations reported, for the integrand f, by $A_1(f), A_2(f), \ldots$, we say that the procedure "converges for f" if

$$\lim_{i\to\infty} A_i(f) = \int_0^1 f(x)\,dx.$$

THEOREM. *There is no adaptive procedure which converges for all functions in* IR.

License or copyright restrictions may apply to redistribution; see https://www.ams.org/journal-terms-of-use

Proof. Suppose the contrary. Let f_1 be twice the characteristic function of $[\frac{1}{2}, 1]$. Since $f_1 \in IR$ and $\int_0^1 f_1 = 1$, there is an integer n_1 such that $A_{n_1}(f_1) > 1/2$. Let S_1 be the set of all those positive values of x at which f_1 was evaluated by the procedure before it reported $A_{n_1}(f_1)$, and let x_1 be the least element of S_1. Define the function g on $[x_1, 1]$ by

$$g(x) = \begin{cases} f_1(x), & x \in S_1, \\ 0, & x \in [x_1, 1] - S_1. \end{cases}$$

Set $g(0) = 0$. We shall later define g on $(0, x_1)$; but however we define it there, it is the case that $A_{n_1}(g) > 1/2$.

Choose numbers b_2 and a_2 such that $0 < a_2 < b_2 < x_1$. Define f_2 by:

$$f_2(x) = \begin{cases} g(x), & x \in [x_1, 1], \\ 1/(b_2 - a_2), & x \in [a_2, b_2], \\ 0, & x \in [0, x_1) - [a_2, b_2]. \end{cases}$$

Thus, $f_2 \in IR$ and $\int_0^1 f_2 = 1$. There is, therefore, an integer $n_2 > n_1$ such that $A_{n_2}(f_2) > 1/2$. Let S_2 be the set of all those positive values of x at which the procedure evaluated f_2 before reporting $A_{n_2}(f_2)$, and let x_2 be a number less than or equal to the least element of S_2 and less than or equal to $x_1/2$. Extend the definition of g to $[x_2, x_1)$ by defining

$$g(x) = \begin{cases} f_2(x), & x \in S_2 \cap [x_2, x_1), \\ 0, & x \in [x_2, x_1) - S_2. \end{cases}$$

Then g and f_2 are equal on S_2, so that $A_{n_2}(g) > 1/2$. Continuing so, we extend the definition of g to $[x_1, 1] \cup [x_2, x_1) \cup [x_3, x_2) \cup \cdots \cup \{0\} = [0, 1]$. At the same time we find a sequence of integers $n_1 < n_2 < n_3 < \cdots$ such that

$$A_{n_i}(g) > 1/2, \qquad i = 1, 2, \ldots .$$

The function g is in IR, and its integral is zero—so the procedure does not converge for g, and the Theorem follows.

The g constructed is discontinuous at infinitely many points, but this is not essential. One could modify the construction along the following lines: Let $t_1 > t_2 > \cdots > t_{m_1}$ be the elements of S_1 and set $t_0 = 1$. For $i \geq 1$, let I_i be an interval of length less than $\min\{1/(5 \cdot 2^i), t_{i-1} - t_i, t_i - t_{i+1}, t_i\}$, centered on t_i. On each I_i, let g be zero at the endpoints and equal to f_1 at t_i; and let g be linear on the right half of I_i and on the left half of I_i. Let $\bar{x}_1 = x_1 - 2^{-m_1-1}$. Then g is defined on $[\bar{x}_1, 1]$, and it remains the case that $A_{n_1}(g) > 1/2$. This g is continuous, and $\int_{\bar{x}_1}^1 g < 1/5$. Similarly modifying the remaining steps of the construction, we can obtain a $g \in IR$ which is continuous on $(0, 1]$ and is such that

$$A_{n_i}(g) > 1/2, \qquad i = 1, 2, \ldots,$$

while $\int_0^1 g < 2/5$.

By "rounding the corners" of the g thus constructed, we could make it as smooth as desired (even C^∞) on $(0, 1]$.

The theorem is perhaps a bit surprising, because of the following considerations:

License or copyright restrictions may apply to redistribution; see https://www.ams.org/journal-terms-of-use

The integral of a function in *IR* is determined, in principle, by the values of the function on any dense set of points, for example, the rationals. An infinitive adaptive procedure can make use of the values of the function at all the rationals. It would seem that the weakest sense that can be given to the phrase "calculate the integral" is the sense used above, in which one asks for a convergent sequence of approximations but does not ask for bounds on the errors of these approximations. We may for the moment call this "A-calculability". Another definition of calculability asks that, for each positive integer n, there be some stage in the calculation at which the integral is definitely known to n significant figures. Let us call this B-calculability; it is equivalent to asking for a sequence $A_1, A_2, \cdots$ of approximations, with associated rigorous error bounds $B_1, B_2, \ldots$, the latter converging to zero. (There are of course other "calculabilities" familiar to numerical analysts. One may ask that the B's be sharp, that $B_n/|A_n - \lim A_n|$ be bounded or even approach 1 as n approaches infinity or that $|A_n - \lim A_n|$, or B_n, go to zero rapidly as some measure of the calculation effort goes to infinity.) Now for the class of functions that are *properly* Riemann-integrable on $[0, 1]$, the integral is A-calculable—the trapezoid rule does it—but it is not B-calculable. That is easy to see directly since even in principle the integral is not determined to any accuracy by the values of the integrand on a finite set of points. Furthermore, it is easy to see that if the proper Riemann-integral were B-calculable, then the improper one that we have dealt with would be A-calculable. However, the improper integral is not A-calculable. The information that determines the integral when it is known all at once does not permit the determination of the integral when it is made known item by item.

Mathematical Analysis Section, IBS
U. S. Department of Commerce
National Bureau of Standards
Washington, D. C. 20234

1. J. R. RICE, *A Metalgorithm for Adaptive Quadrature*, CSDTR89, Purdue University, March, 1973.

2. P. J. DAVIS & P. RABINOWITZ, "Ignoring the singularity in approximate integration," *J. Soc. Indust. Appl. Math. Ser. B Numer. Anal.*, v. 2, 1965, pp. 367–383. MR 33 #3459.

License or copyright restrictions may apply to redistribution; see https://www.ams.org/journal-terms-of-use