Handheld Calculator Evaluates Integrals

The HP-34C is the first handheld calculator to have a key that performs numerical integration almost automatically. It may change your attitude towards what used to be regarded as a dreary tedious task.

by William M. Kahan

NUMERICAL INTEGRATION has been the subject of about two thousand books and learned papers, with a dozen or so "new" methods published every year. And yet the task in question has a simple geometrical interpretation seen in Fig. 1: given an expression f(u) and lower and upper limits y and x respectively, the value

$$I = \int_y^x f(u)\,du$$

represents the area under the graph of f(u) for u between y and x. Why so much fuss?

As I write this an electrical engineering colleague, Professor J. R. Woodyard, enters my office and asks to have

$$I_1 = \int_0^1 \left(\frac{\sqrt{u}}{u-1} - \frac{1}{\ln u} \right) du$$

evaluated on my HP-34C Calculator (Fig. 2). Let's do it.

Step 1. Key into the calculator under, say, label **A** a program that accepts a value u in the display (X register) and displays instead the computed value of the integrand

$$\sqrt{u}/(u-1) - 1/(\ln u)$$

Fig. 3 shows an HP-34C program to do this.

Step 2. Restore the calculator to **RUN** mode and set the display to, say, **FIX 5** to display five decimal digits after the point, which are as many digits of the integrand as my client says he cares to see. (More about this later.)

Step 3. Key in the lower and upper limits of integration thus, **0 ENTER↑ 1**, thereby putting 0 into the Y register and 1 into X.

Step 4. Press $\int_y^x$ **A**, wait 25 seconds until the display shows 0.03662, then press **x≶y** to see 0.00001. We have just calculated

$$I_1 = 0.03662 \pm 0.00001.$$

That was easy—too easy. Woodyard smiles as if he knew something I don't know. Could the calculator be wrong? How does the calculator know the error lies within ±0.00001?

Many other questions come to mind:

- Why is numerical integration impossible in general?
- Why do we persist in trying to do it anyway?
- How do we do it? How well do we do it?
- How does the $\int_y^x$ key compare with other integration schemes?
- What can go wrong and how do we avoid it?
- What else have we learned?

These questions and others are addressed in the following pages.

Tolerance and Uncertainty

Integrals can almost never be calculated precisely. How much error has to be tolerated? The $\int_y^x$ key answers this question in a surprisingly convenient way. Rather than be told how accurately $I = \int_y^x f(u)du$ should be calculated, the HP-34C asks to be told how many figures of f(u) matter. In effect, the user is asked to specify the width of a ribbon drawn around the graph of f(u), and to accept in place of I an estimate of the area under some unspecified graph lying entirely within that ribbon. Of course, this estimate could vary by as much as the area of the ribbon, so the calculator estimates the area of the ribbon too. Then the user may conclude from Fig. 4 that

I = (area under a graph drawn in the ribbon)
± (½ area of the ribbon)

The calculator puts the first area estimate in its X register and the second, the uncertainty, in the Y register.

For example, f(u) might represent a physical effect whose magnitude can be determined only to within, say, ±0.005. Then the value calculated as f(u) is really f(u) ± Δf(u) with an uncertainty Δf(u) = 0.005. Consequently **FIX 2**, which tells the calculator to display no more than two decimal digits after the point, is used to tell the calculator that decimal digits beyond the second cannot matter. Therefore the calculator need not waste time estimating $I \pm \Delta I = \int_y^x (f(u) \pm \Delta f(u))du$ more accurately than to within an uncertainty $\Delta I = \left|\int_y^x \Delta f(u)du\right|$. This uncertainty is estimated together with $I \pm \Delta I$, thereby giving the calculator's user a fair idea of the range of values within which I must lie.

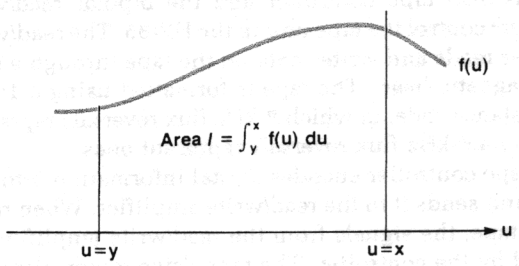

Fig. 1. *An integral interpreted as an area.*

Fig. 2. *HP-34C Calculator has keys to solve any equation and to compute integrals.*

The uncertainty Δf(u) is specified by the user via the display setting. For instance, **SCI 5** displays six significant decimal digits, implying that the seventh doesn't matter. The HP-34C allows the user's f-program to change the display setting, thereby providing for uncertainties Δf(u) that vary with u in diverse ways. But users usually leave the display set to **SCI 4** or **FIX 4** without much further thought.

By asking the user to specify Δf(u) instead of Δ*I* the HP-34C helps avoid a common mistake—wishful thinking. Other integration procedures, which conventionally expect the user to specify how tiny Δ*I* should be, blithely produce estimates of *I* purporting to be as accurate as the user wishes even when the error Δf(u) is far too big to justify such claims to accuracy. The HP-34C does not prevent us from declaring that f(u) is far more accurate that it really is, but our attention is directed to the right question and not distracted by questions we cannot answer. Whether we specify Δf after a careful error analysis or just offer a guess, we get estimates $I \pm \Delta I$ that we can interpret more intelligently than if we got only *I* with no idea of its accuracy or inaccuracy.

A Survey of Integration Schemes

Students are taught the fundamental theorem of calculus:

$$I = \int_y^x f(u)\,du = F(x) - F(y) \quad \text{provided } \frac{d}{du} F(u) = f(u)$$

This means that one could calculate *I* if one could discover somehow an expression F(u) whose derivative is the given expression f(u). Students are taught integration as a process, applied to expressions, that starts with f and ends with F. But in professional practice that process hardly ever succeeds. A compact expression F(u) is almost always difficult or impossible to construct from any given f(u). For instance, neither

$$\int_{-\infty}^{x} \exp(-u^2/2)du/\sqrt{2\pi} \quad \text{nor} \quad \int_0^{\infty} \exp(-u + x \ln u)du$$

possesses a closed form, that is, an expression involving only finitely many elementary operations (+, −, ×, ÷, ln, exp, tan, arctan, ...) upon the variable x. Nevertheless, both integrals can be approximated arbitrarily accurately by aptly chosen formulas. So often do statisticians and engineers need values of those integrals that formulas for them, accurate to ten significant decimal digits, can now be calculated in a few seconds by pressing a key on certain handheld calculators. (Press **Q** on the HP-32E to get the first integral, the cumulative normal distribution; press **x!** on the HP-34C to get the second integral, the gamma function Γ(1+x), whether x be an integer or not.)

Almost every rare integrand f(u) whose indefinite integral $F(x) = \int^x f(u)du + c$ is expressible in a compact or closed form can be recognized by a computer program that accepts the string of characters that defines f and spews out another string that represents F. (Such a program is part of the MACSYMA system, developed at MIT, that runs on a few large computers—two million bytes of memory—at several universities and research labs.) Perhaps the terms "compact" and "closed form" should not be attached to the expression F(x), since usually, except for problems assigned to students by considerate teachers, the integral

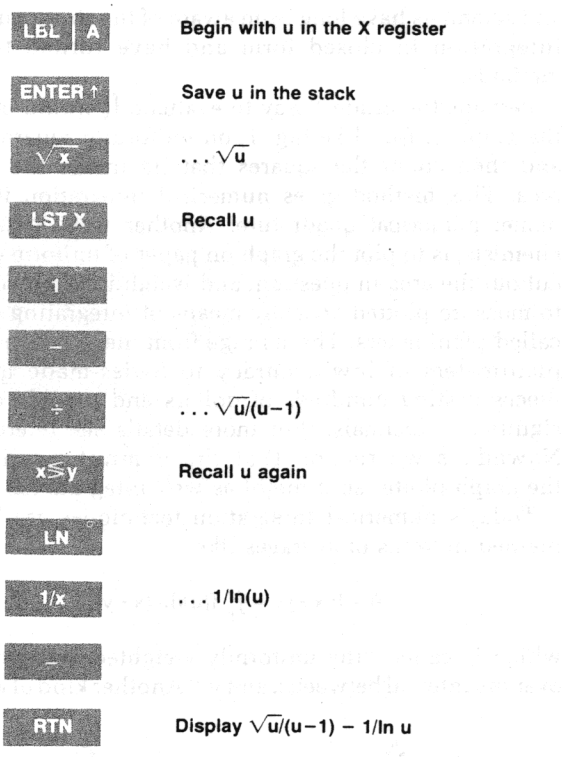

Fig. 3. *This program makes the HP-34C calculate the integrand $\sqrt{u}/(u-1) - 1/\ln u$ when the argument u is in the X register and key **A** is pressed. Labels B, 0, 1, 2, or 3 would have served as well as A.*

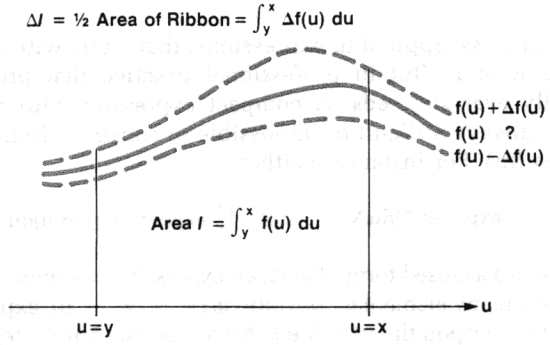

Fig. 4. *The graph of an uncertain integrand f(u) ±Δf(u) can run anywhere in the ribbon bounded by the dashed lines. The area under such a graph, I ±ΔI, is uncertain by ±ΔI, which is one-half the area of the ribbon. The HP-34C displays its estimate of I ±ΔI in its X register and holds an estimate of ΔI in its Y register.*

F(x) far exceeds the integrand f(u) in length and complexity. Shown in Fig. 5 are two compact forms and one closed form for F(x) when $f(u) \equiv 1/(1+u^{64})$. The extent to which F(x) is here more complicated than f(u) is atypically modest out of consideration for the typesetter. The formulas in Fig. 5 will remind many readers of hours spent on calculus problems, but they do not provide economical ways to calculate F(x) for any but very big or very tiny values of x. When I use the HP-34C's $\int_y^x$ key to calculate $F(1) = \int_0^1 du/(1+u^{64}) = 0.989367 \pm 0.000004$ the answer appears in 200 seconds including 20 seconds taken to enter the f-program plus 180 seconds for a result (in **SCI 5**). Calculating F(1) from any formula in Fig. 5 takes at least about ten times longer, not including the time taken to deduce the formula. Engineers and scientists have long been aware of the shortcomings of integration in closed form and have turned to other methods.

Perhaps the crudest way to evaluate $\int_y^x f(u)du$ is to plot the graph of f(u), like Fig. 1, on uniformly squared paper and then count the squares that lie inside the desired area. This method gives numerical integration its other name: numerical quadrature. Another way, suitable for chemists, is to plot the graph on paper of uniform density, cut out the area in question, and weigh it. Engineers used to measure plotted areas by means of integrating engines called planimeters. These range from inexpensive hatchet planimeters of low accuracy to Swiss-made museum pieces costing hundreds of dollars and capable of three significant decimals. (For more details see reference 1). Nowadays we reckon that the computer will drive the graph plotter so it might as well integrate too.

Today's numerical integration techniques are best explained in terms of averages like

$$A = I/(x-y) = \int_y^x f(u)du/(x-y)$$

which is called "the uniformly weighted average of f(u) over the interval between x and y." Another kind of average,

$$A = \sum_{j=1}^{n} w_j f(u_j) \quad \text{where} \quad w_j > 0 \text{ and } \sum_{j=1}^{n} w_j = 1,$$

is a finite weighted average of n samples $f(u_1), f(u_2), \ldots, f(u_n)$. Provided the sample arguments $u_1, u_2, \ldots, u_n$, called nodes, all lie between x and y the sample average A will approximate, perhaps poorly, the desired average A, and hence provide $I = (x-y)A$ as an approximation to $I = (x-y)A$. Statisticians might be tempted to sprinkle the nodes u_j randomly between x and y—that is what Monte Carlo methods do. But randomness is a poor substitute for skill because the error $A-A$ tends to diminish like $1/\sqrt{n}$ as the number n of random samples is increased, whereas uniformly spaced and weighted samples provide an error that diminishes like $1/n^2$. Other more artful methods do even better.

Different numerical integration methods differ principally in the ways they choose their weights w_j and nodes u_j, but almost all have the following characteristics in common. Each average A is associated with a partition of the range of integration into panels as shown in Fig. 6. Each panel contains one node u_j whose respective weight is

w_j = (width of panel j)/(width of range of integration).

The formula given above for A amounts to approximating the area in each panel under the graph of f(u) by the area of a rectangle as wide as the panel and as high as the sample $f(u_j)$. The simplest method is the midpoint rule, whose nodes all lie in the middles of panels all of the same width. Other methods, like the trapezoidal rule and Simpson's rule, vary the panel widths (weights) and nodes in ways designed to exploit various presumed properties of the integrand f(u) for higher accuracy. Which method is best? If this question had a simple answer there would not be so many methods nor would we need texts like "Methods of Numerical Integration" by P.J. Davis and P. Rabinowitz,[2] which contains 16 FORTRAN programs and three bibliographies with well over 1000 citations.

For example, consider Gaussian quadrature. This method is widely regarded as "best" in the sense that it very often requires fewer samples than most other methods to achieve an average A that approximates the desired A to within some preassigned tolerance. But the weights and nodes of Gaussian quadrature take quite a while to calculate. Programs to do so, and the resulting tables of weights and nodes for various sample counts n, have been published.[3] Had we chosen Gaussian quadrature for the $\int_y^x$ key we would

$$F(x) \equiv \int_0^x f(u)\,du \quad \text{where} \quad f(u) \equiv 1/(1+u^{64}).$$

$$F(x) = x \sum_{k=0}^{\infty} (-x^{64})^k / (64k+1) \quad \text{if} \quad x^2 \leq 1$$

$$= \frac{\pi}{64} \csc\left(\frac{\pi}{64}\right) \operatorname{sign}(x) + x \sum_{k=1}^{\infty} (-x^{-64})^k / (64k-1) \quad \text{if} \quad x^2 \geq 1$$

$$= \frac{1}{32} \sum_{k=1}^{16} \left(\sin\theta_k \cdot \arctan\left(\frac{2x\sin\theta_k}{1-x^2}\right) + \tfrac{1}{2}\cos\theta_k \cdot \ln\left(1 + \frac{2}{\frac{x+x^{-1}}{2\cos\theta_k} - 1}\right) \right)$$

$$+ \left(\frac{\pi}{64} \csc\left(\frac{\pi}{64}\right) \operatorname{sign}(x) \quad \text{if} \quad x^2 > 1\right) \qquad \text{where } \theta_k = (k-\tfrac{1}{2})\pi/32$$

Fig. 5. *Formal integration transforms many a simple expression f(u) into messy formulas F(x) of limited numerical utility.*

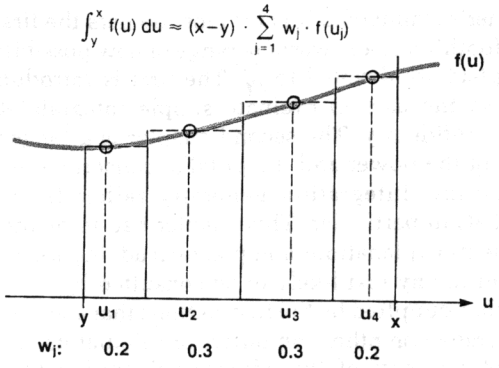

Fig. 6. *The integral, regarded as an area, is here divided into four panels each of whose areas is approximated by the area of a rectangle as wide as the panel and as high as a sample.*

have had to store at least as many nodes and weights as we could expect to need for difficult integrals, amounting to at least several hundred 13-digit numbers, in read-only memory. But that would have left no space in the HP-34C for anything else, so a different method had to be found.

The $\int_y^x$ key could not use a method that generates just one average A because that gives no indication of how accurately it approximates A. Instead we looked only at methods that sample repeatedly and with increasing sample counts $n_1 < n_2 < n_3 < \ldots$ to produce a sequence of increasingly accurate averages $A_1, A_2, A_3, \ldots$. Provided that sequence converges to A so fast that each $|A_{k+1} - A|$ is considerably smaller than its predecessor, the error $|A_k - A|$ can be approximated accurately enough by $|A_k - A_{k+1}|$, and the last average A_{k+1} can be accepted in lieu of A as soon as $|A_k - A_{k+1}|$ is tolerably small.

How small is "tolerably small"? That depends upon the area of the ribbon discussed above under "Tolerance and Uncertainty." Since the integral $I = \int_y^x f(u)du$ inherits an uncertainty $\Delta I = \left| \int_y^x \Delta f(u)du \right|$ from the uncertainty $\Delta f(u)$ in the integrand, so does $A = I/(x-y)$ inherit an uncertainty $\Delta A = \Delta I/|x-y|$, which may be approximated by

$$\Delta A = \sum_{j=1}^{n} w_j \Delta f(u_j)$$

in the same way as A is approximated by A. Indeed, A and ΔA can be computed together since they use identical weights and nodes. And so the sequence $A_1, A_2, A_3, \ldots$ is accompanied by a sequence of respective uncertainty estimates $\Delta A_1, \Delta A_2, \Delta A_3, \ldots$. Now "tolerably small" can be defined to mean "rather smaller than ΔA_{k+1}."

The foregoing argument provides an excuse for accepting A_{k+1} in lieu of A whenever two consecutive estimates A_k and A_{k+1} agree to within ΔA_{k+1}, but it provides no defense against the possibility that convergence is not so fast, in which case A_k and A_{k+1} might agree by accident and yet be both quite different from A. The $\int_y^x$ key waits for three consecutive estimates A_k, A_{k+1}, and A_{k+2} to agree within ΔA_{k+2}. Only the most conservative integration schemes wait that long. While this conservatism strongly attenuates the risk of accidental premature acceptance of an estimate, the risk that three consecutive estimates might agree within the tolerance and yet be quite wrong cannot be eliminated. Later, under "How to Deceive Every Numerical Integration Procedure," some such risk will be proved unavoidable, but the risk now is so small that further attenuation is not worth its cost.

The combination of ignorance with conservatism is surprisingly costly. Had we known in advance that A_k would be accurate enough we would have calculated none of the other averages. Instead, waiting for three consecutive averages to agree could easily cost some methods almost 6.25 times as many samples as if only A_k had to be calculated, and more than that if the sample counts n_1, n_2, n_3, ... are not chosen optimally. For the $\int_y^x$ key we chose $n_k = 2^k - 1$ and we chose a method whose successive averages each share almost half of the previous average's samples, thereby preventing the cost of ignorance from much exceeding a factor of 4.

Memory limitations precluded the use of another family of methods known as adaptive quadrature. These methods attempt to distribute nodes more densely where the integrand f(u) appears to fluctuate rapidly, less densely elsewhere where f(u) appears to be nearly constant or relatively negligible. They succeed often enough that the best general-purpose integrators on large computers are adaptive programs like Carl de Boor's CADRE; this and others are described in reference 2. Alas, adaptive programs consume rather more memory for scratch space than the twenty registers available in the HP-34C.

What Method Underlies the $\int_y^x$ Key?

The HP-34C uses a Romberg method; for details consult reference 2. Several refinements were found necessary. Instead of uniformly spaced nodes, which can induce a kind of resonance or aliasing that produces misleading results when the integrand is periodic, the $\int_y^x$ key's nodes are spaced nonuniformly. Their spacing can be explained by substituting, say,

$$u = \frac{3}{2}v - \frac{1}{2}v^3$$

into

$$I = \int_{-1}^{1} f(u)du = \int_{-1}^{1} f\left(\frac{3}{2}v - \frac{1}{2}v^3\right)\cdot\frac{3}{2}(1-v^2)dv$$

and distributing nodes uniformly in the second integral. Besides suppressing resonance, the substitution confers two more benefits. One is that no sample need be drawn from either end of the interval of integration, except when the interval is so narrow that no other possibilities are available, and consequently an integral like

$$\int_0^3 \frac{\sin u}{u}\,du$$

won't hang up on division by zero at an endpoint. Second, $I = \int_y^x f(u)du$ can be calculated efficiently when $f(u) = g(u)\sqrt{|x-u|}$ or $g(u)\sqrt{(x-u)(u-y)}$ where g(u) is everywhere a smooth function, without any of the expedients that would otherwise be required to cope with the infinite values taken by the derivative f'(u) at u = x or u = y. Such integrals are encountered often during calculations of areas enclosed by smooth closed curves. For example, the area of a circle of radius 1 is

$$\int_0^2 \sqrt{u(4-u)}du = 3.14159 \pm 8.8\times10^{-6}$$

which consumes only 60 seconds when evaluated in **SCI 5** and only 110 seconds to get $3.141592654\pm1.4\times10^{-9}$ in **SCI 9**.

Another refinement is the use of extended precision, 13 significant decimal digits, to accumulate the sums that define A_k, thereby allowing thousands of samples to be accumulated, if necessary, without losing to roundoff any more information than is lost within the user's own f-program. The last example's 10 significant decimal digits of π could not have been achieved without such a refinement.

How Does the $\int_y^x$ Key Compare with Other Integrators?

What most distinguishes the HP-34C's $\int_y^x$ key from all other schemes is its ease of use. No step-size parameters, no plethora of error tolerances, no warning indicators that "can usually be ignored." Only the minimum information needed to specify $\int_y^x (f(u)\pm\Delta f(u))du$ has to be supplied. And because the $\int_y^x$ key is effective over so wide a range of integrals it ranks among the most reliable procedures available anywhere. Usually it is far faster than simpler procedures like the trapezoidal rule or Simpson's rule commonly used previously on calculators. For integrands defined by programs that fit comfortably into a mid-sized handheld calculator that can hold at most 210 program steps, the $\int_y^x$ key is comparable in speed (count the number of samples) with the integrators available on large computers. For much more complicated integrands the best adaptive integrators on large computers are appreciably faster.

One of the HP-34C's most important components is its Owner's Handbook. It is for most owners the first guide to the foothills of an awesome range of new possibilities. Two chapters are devoted to $\int_y^x$. The first is introductory, and allows the user to evaluate simple integrals effortlessly and confidently. The second chapter is a longer explanation of the power and the pitfalls, concerned mainly with numerical integration generally rather than with the HP-34C in particular. This chapter had to be included because its explanations and practical advice are not yet to be found in any text likely to be consulted by an owner, nor are they supplied by the instructions that accompany other integrators on other computers or calculators. This second chapter is part of the educational burden that must be borne by innovators and pioneers. The Owner's Handbook provides no formulas for the nodes and weights used by the HP-34C because they are not needed to understand how the $\int_y^x$ key works; instead they can be deduced from information in this article.

Every numerical integrator like $\int_y^x$, which executes a user-supplied program to get the integrand's value f(u), imposes constraints upon that program. Some constraints, like requiring f to have a smooth graph on the interval of integration, are practically unavoidable. Others are nuisances like

- Begin the f-program with a special label, say A′.
- Do not use certain memory registers, say #0 - #5.
- Do not use certain operations, say = and **CLR**.

The $\int_y^x$ key is encumbered with no such nuisances. The f-program may begin with any of several labels, so several different integrals can be calculated during one long computation. The f-program may use memory registers freely and may use any operation key except $\int_y^x$ itself. One of

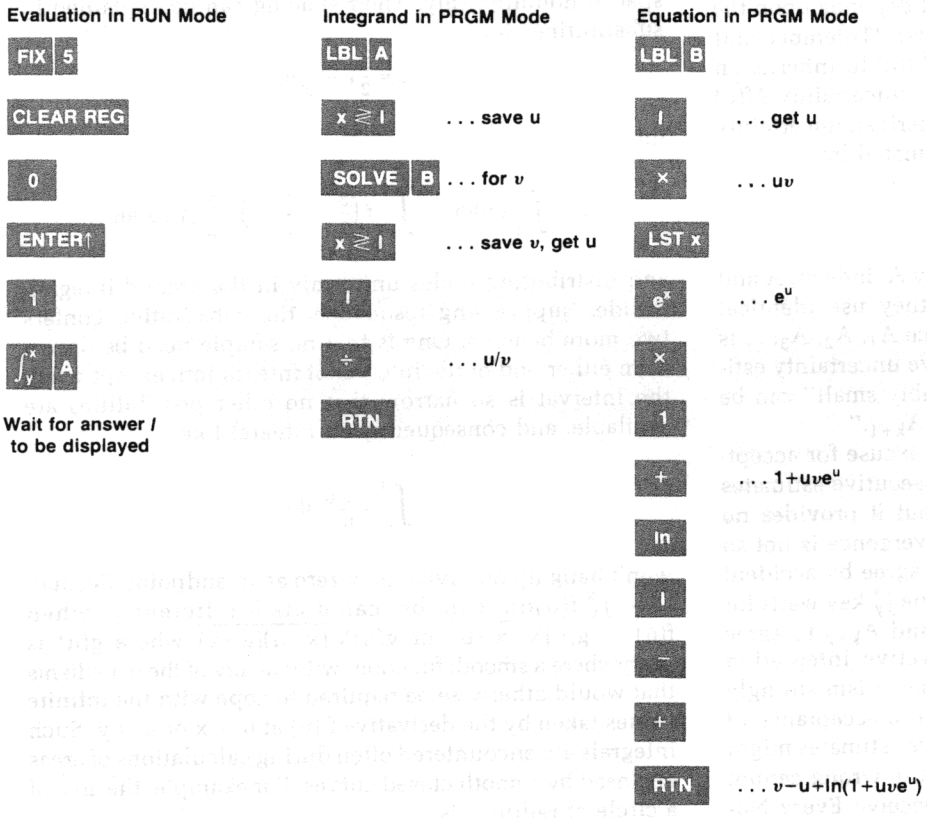

Fig. 7. *A program to evaluate* $I = \int_0^1 udu/v(u)$ *where* $v = v(u)$ *satisfies* $v-u+ln\,(1+uve^u)=0$.

those keys is the HP-34C's powerful **SOLVE** key.[4] Consequently this calculator is currently the only one that can evaluate conveniently integrals of implicit functions.

For example, let $v = v(u)$ be the root of the equation

$$v - u + \ln(1 + uve^u) = 0.$$

Then

$$\int_0^1 u\, du/v(u) = 1.81300 \pm 0.000005$$

results from a program rather shorter than on any previous calculator; it is exhibited in Fig. 7.

Furthermore, $\int_y^x$ may be invoked, like any other function, from within a program, thereby permitting the HP-34C to **SOLVE** equations involving integrals. For example, solving

$$\int_0^\pi \cos(x \sin\theta)d\theta = 0$$

for $x = 2.405...$ takes a short program contained in the Owner's Handbook, and exhibits the first zero of the Bessel function $J_0(x)$.

How to Deceive Every Numerical Integration Procedure

Such a procedure must be a computer program—call it P—that accepts as data two numerical values x and y and a program that calculates f(u) for any given value u, and from that data P must estimate $I = \int_y^x f(u)\, du$. The integration procedure P is not allowed to read and understand the f-program but merely to execute it finitely often, as often as P likes, with any arguments u that P chooses. What follows is a scheme to deceive P.

First ask P to estimate I for any two different values x and y and for $f(u) \equiv 0$. Record the distinct arguments $u_1, u_2, ..., u_n$ at which P evaluates f(u). Presumably when P finds that $f(u_1) = f(u_2) = ... = f(u_n) = 0$ it will decide that $I = 0$ and say so. Next give P a new task with the same limits x and y as before but with a different integrand

$$f(u) \equiv ((u-u_1)\cdot(u-u_2)\cdot...\cdot(u-u_n))^2.$$

Once again P will calculate $f(u_1)$, $f(u_2)$, ..., and finding no difference between the new f and the old, P will repeat exactly what it did before. But the new integral I is quite different from the old, so P must be deceived.

The HP-34C's $\int_y^x$ key can be hoodwinked that way. Try to evaluate $\int_{-128}^{+128} f(u)du$ using first $f(u) \equiv 0$ programmed in a way that pauses (use the **PSE** key) to display its argument u. The calculator will display each sample argument it uses, namely 0, ±88, ±47 and ±117. Next program

$$f(u) \equiv (u(u-88)(u+88)(u-47)(u+47)(u-117)(u+117))^2$$

and evaluate $\int_{-128}^{+128} f(u)du$ again. The calculator will say that both integrals are 0, but the second polynomial's integral is really 1.310269×10^{28}. That polynomial's graph, shown in Fig. 8, has the sharp spikes that characterize integrands troublesome for every numerical integration procedure. To calculate the integral correctly, reevaluate it as $2\int_0^{128} f(u)du$, thereby doubling the spikes' width compared with the range of integration.

The threat of deceit impales the designer of a numerical integrator upon the horns of a dilemma. We all want our integrators to work fast, especially when the integrand f(u) is very smooth and simple like $f(u)=3u-4$. But if the integrator is too fast it must be easy to deceive; fast integration means few samples $f(u_j)$, implying wide gaps between some samples, which leave room for deceitful misbehavior. Figs. 9a-9e illustrate the dilemma with two estimates of $\int_y^x f(u)du$. The first estimate is based upon the three samples drawn at the white dots, the second upon seven samples including those three white plus four more black dots. Fig. 9a shows why all sufficiently smooth graphs f(u) that agree at all seven samples have nearly the same integrals, but Fig. 9b shows how two integrands could provide the same samples and yet very different integrals. The coincidence in Fig. 9b is unlikely; successive estimates based upon increasingly dense sampling normally would reveal the difference as in Fig. 9c. However, situations like those illustrated in Figs. 9d and 9e are very likely to deceive.

Textbooks tell us how to avoid being deceived: avoid integrands f(u) among whose first several derivatives are some that take wildly different values at different places in the range of integration. Or avoid integrands f(u) that take wildly different values when evaluated at complex arguments in some neighborhood of the range of integration. And if wild integrands cannot be avoided they must be tamed. We shall rejoin this train of thought later.

Improper and Nearly Improper Integrals

An improper integral is one that involves ∞ in at least one of the following ways:

- One or both limits of integration are ±∞, e.g.,

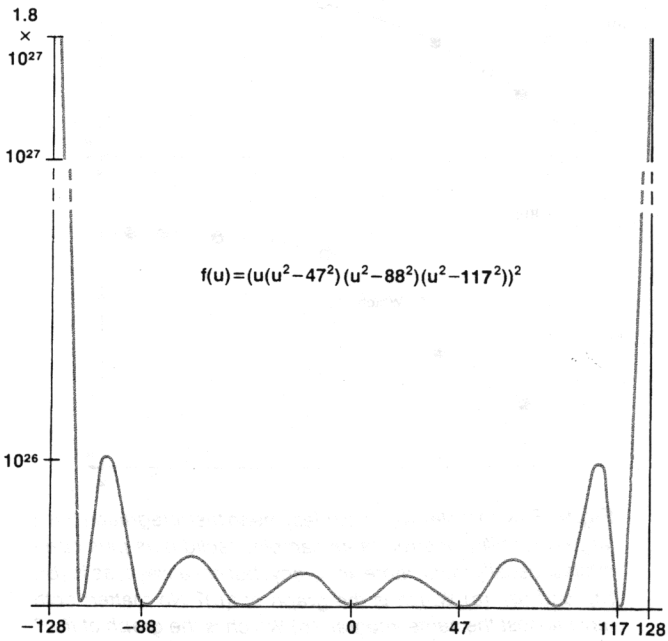

Fig. 8. *The polynomial f(u) was devised to deceive the HP-34C into miscalculating its integral as 0 instead of 1.31×10^{28}. This spiky graph is typical of integrands that can baffle any numerical integrator. 73% of the area under the graph lies under two spikes whose widths span less than 4% of the area of integration.*

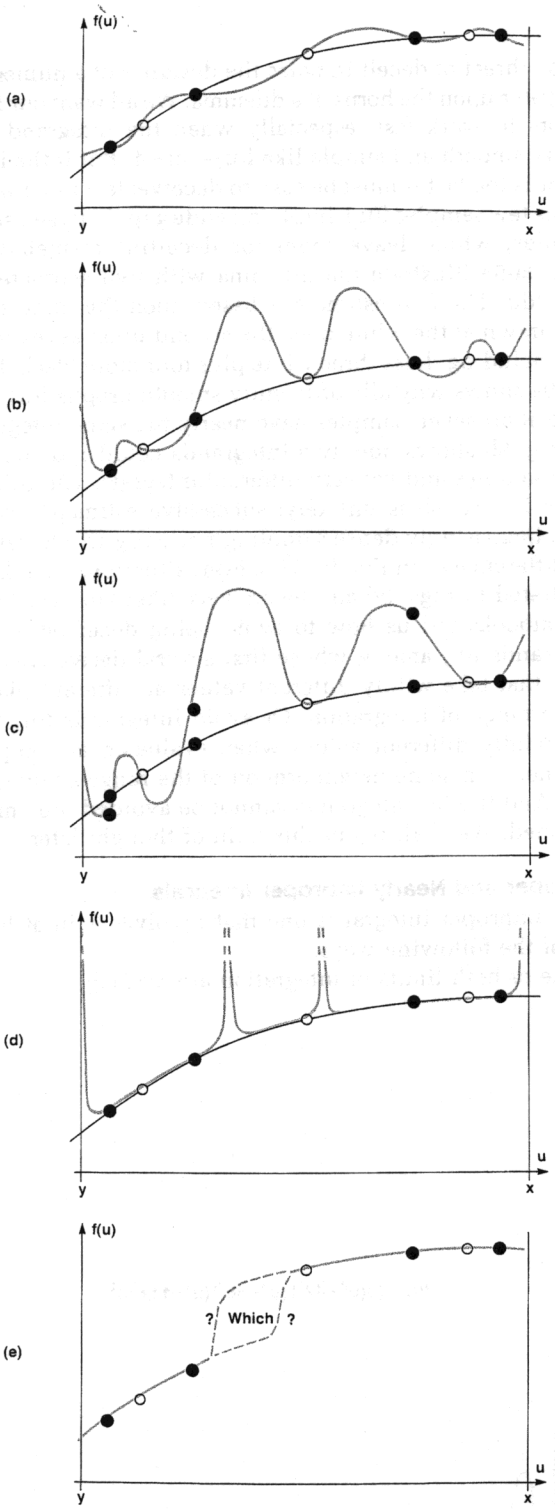

Fig. 9. *Few samples (open circles) mean fast integration but a large possibility of error. More samples (solid dots plus open circles) usually mean more accuracy, but not always, as in (b), (d), and (e). (a) Which is the graph of f(u)? No matter; both have almost the same integral. (b) Which is the graph of f(u)? They have very different integrals. (c) Here two graphs that coincide on the first samples ○ are distinguished by a significantly different outcome after second samples ● are drawn. (d) If the graph of f(u) has a few sharp and narrow spikes, they will probably be overlooked during the estimation of the integral based on finitely many samples. (e) If the graph of f(u) has a step that was not made known during the estimation of the integral, then the estimate may be mistaken.*

$$\int_{-\infty}^{\infty} \exp(-u^2)\,du = \sqrt{\pi}/2.$$

- The integrand tends to $\pm\infty$ someplace in the range of integration, e.g.,

$$\int_0^1 \ln(u)du = 1.$$

- The integrand oscillates infinitely rapidly somewhere in the range of integration, e.g., $\int_0^1 \cos(\ln u)du = 1/2$.

Improper integrals are obviously troublesome. Equally troublesome, and therefore entitled to be called nearly improper, are integrals afflicted with the following malady:

- The integrand or its first derivative changes wildly within a relatively narrow subinterval of the range of integration, or oscillates frequently across that range.

This affliction can be diagnosed in many different ways. Sometimes a small change in an endpoint can render the integral improper, as in

$$\int_{0.0001}^1 \ln(u)du = -0.99898\ldots \rightarrow \int_0^1 \ln(u)du = 1.$$

Sometimes a small alteration of the integrand can render the integral improper, as in

$$\int_{-1}^1 dx/(x^2 + 10^{-10}) = 314157.2654\ldots \rightarrow \int_{-1}^1 dx/x^2 = \infty.$$

Sometimes the value of the integral is nearly independent of relatively huge variations in one or both of the endpoints, as is $\int_0^x \exp(-u^2)\,du \approx \sqrt{\pi}/2$ for all $x > 10$. Regardless of the cause or diagnosis, nearly improper integrals are the bane of numerical integration programs, as we have seen.

During the HP-34C's design a suspicion arose that most integrals encountered in practice might be improper or nearly so. Precautions were taken. Now that experience has confirmed the suspicion, we are grateful for those precautions. They were:

1. Avoid sampling the integrand at the ends of the range of integration.
2. By precept and example in the Owner's Handbook, warn users against wild integrands, suggest how to recognize them, and illustrate how to tame them.

The second precaution ignited controversy. Against it on one side stood fears that its warnings were excessive and might induce paranoia among potential customers. Who would buy a calculator that he thinks gets wrong answers? Actually wrong answers were very rare, thanks in part to the first precaution, and many attempts to vindicate dire predictions about mischievous improper and nearly improper integrals were thwarted by unexpectedly correct answers like

$$\int_0^1 \ln(u)\,du = 0.9998 \pm 0.00021$$

in 2 minutes at **SCI 3**. Or

$$\int_0^{30} \exp(-u^2)\,du = 0.886227 \pm 0.0000008$$

in 4 minutes at **SCI 5**. If the wages of sin be death, O Death, where is thy sting?

On the other side stood a number of embarrassing examples like

$$\int_0^{400} \exp(-u^2)\, du$$

miscalculated as 0.0 ± 0.0000000005 in 14 seconds. Another, had we known it then, would have been Woodyard's example at the beginning of this article; the correct answer

$$\int_0^1 \left(\frac{\sqrt{u}}{u-1} - \frac{1}{\ln u} \right) du = 0.03649 \pm 0.00000007$$

in 23 minutes at **FIX 7** differs from **FIX 5**'s wrong answer 0.03662 in the worst way; the error is too small to be obvious and too large to ignore. Adding to the confusion were examples like

$$A(x) = x^{-1} \int_0^x \sqrt{-2 \ln \cos(u^2)}\, du/u^2 = 1 + x^4/60 + x^8/480 + \ldots$$

for which computation in **SCI 4** produced ridiculous values like $A(0.1) = 0.95742 \pm 0.00005$, $A(0.01) = 0.58401 \pm 0.00003$, and $A(0.001) = 0$, all impossibly smaller than 1. This example appears to condemn the $\int_y^x$ key until the integrand $f(u)=\sqrt{-2 \ln \cos(u^2)}/u^2$ is watched for small arguments u and seen to lose most of its figures to roundoff, losing all of them for $|u| \leq 0.003$, despite an absence of subtractions that could be blamed for cancellation. Then the example appears to condemn the whole calculator. Who wants responsibility for a calculator that gets wrong answers?

Don't panic! The answers are wrong but the calculator is right.

How to Tame a Wild Integral

Forewarned is forearmed. Every experienced calculator user expects to encounter pathological examples like some of those above, and expects to cope with them. The question is not "whether" but "when"? And that is when attention to detail by the calculator's designers is rewarded by the user's freedom from petty distractions that can only complicate a task already complicated enough. But like the dog that did not bark,* the absence of distracting details may fail to be appreciated. That is why the examples explained below have been chosen—to illustrate the advantages of liberated thought. Work them on your calculator as you read them; don't skim them like a novel. Then you may come to think of your calculator the way I think of mine, as a trusted friend who stays with me when I need help.

The integral $A(x)$ above contains an integrand $f(u) = \sqrt{-2 \ln \cos(u^2)}/u^2$ that loses its figures when u becomes tiny. The problem is caused by rounding $\cos(u^2)$ to 1, which loses sight of how small u^2 must have been. The solution compensates for roundoff by calculating f(u) as follows:

Let $y = \cos u^2$ rounded.
If $y = 1$ then let $f(u) = 1$
else let $f(u) = \sqrt{-2 \ln y}/\cos^{-1} y$.

The test for $y = 1$ adds four steps to the f-program and, provided ln and $\cos^{-1}$ are implemented as accurately as on all recent HP calculators, the problem goes away.

*See the last few paragraphs of the Sherlock Holmes story "Silver Blaze" by Conan Doyle.

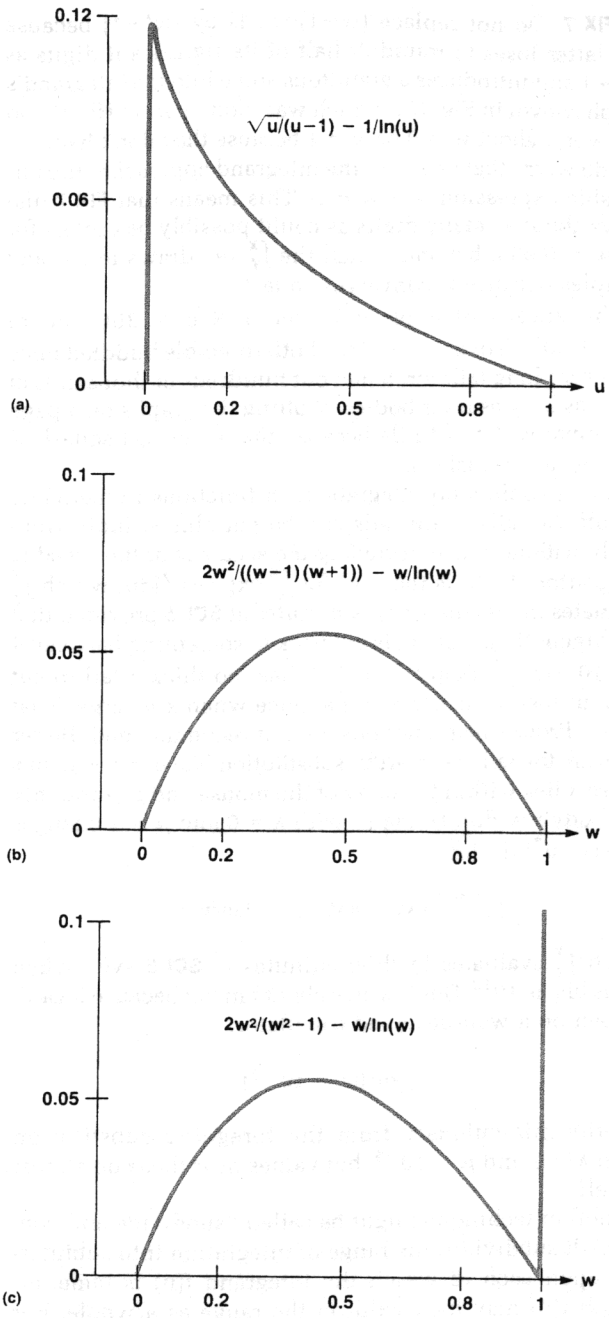

Fig. 10. *Substituting w^2 for u turns the wild graph (a) into the easy one (b). But do not replace ((w−1) (w+1)) by (w^2-1) because roundoff errors introduce a spike, as shown in (c).*

Woodyard's example I_1 has an integrand f(u) whose derative $f'(u) \to \infty$ as $u \to 0$. The graph of f(u) shown in Fig. 10a looks like a lovers' leap. Stretching the u-axis near u=0 by substituting $u = w^2$ turns the precipice into the hummock shown in Fig. 10b and transforms the integral into an easy calculation:

$$I_1 = \int_0^1 \left(\frac{2w^2}{(w-1)(w+1)} - \frac{w}{\ln w} \right) dw$$

The HP-34C computes this as 0.03649 ± 0.000005 in 100 seconds at **FIX 5** or 0.0364900 ± 0.00000008 in 200 seconds

at **FIX 7**. Do not replace $(w-1)(w+1)$ by (w^2-1) because the latter loses to roundoff half of its significant digits as $w \to 1$ and introduces a gratuitous spike into the integrand's graph shown in Fig. 10c, which was plotted on an HP-85. Do not worry about $w = 0$ or $w = 1$ because they don't happen, but do worry that as $w \to 1$ the integrand approaches the unreliable expression $\infty - \infty = 0$. This means that **FIX 7** displays about as many digits as could possibly be correct for all $w < 0.999$, beyond which the $\int_y^x$ key draws few if any samples because it converges so fast.

The graphs of $\exp(-u^2)$ over $0 \leq u \leq 300$ and of $1/(u^2 + 10^{-10})$ over $-1 \leq u \leq 1$ both resemble huddled mice with very long tails stretched out hundreds or thousands of times as long as their bodies. Plotting the graphs on a page of normal width is futile because the bodies get squashed into vertical whiskers.

Most people who integrate such functions numerically cut off the tails. Thin tails can be cut almost indiscriminately without much degrading the accuracy or the speed of integration. Such is the case for $\int_0^x \exp(-u^2)du$, which $\int_y^x$ evaluates in less than, say, 4 minutes at **SCI 5** provided that x, if bigger than 4 or 10, is cut back to something between 4 and 10. But $\int_{-x}^{x} du/(u^2 + 10^{-10})$ has too thick a tail to cut without losing accuracy or patience when x is large. That is why Procrustean methods are not recommended. Better to shrink the tail via an artful substitution like $u = \lambda + \mu\tan v$ where λ lies within the body of the mouse and μ is roughly that body's width. Doing so with $\lambda = 0$ and $\mu = 1$ changes $\int_0^x \exp(-u^2)\, du$ into

$$\int_0^{\arctan x} \exp(-\tan^2 v)\,(1 + \tan^2 v)\, dv$$

which $\int_y^x$ evaluates in three minutes at **SCI 5** even when x is as big as 10^{10}. Don't worry about $\tan \pi/2$ because it can't happen on a well-designed calculator.

$$\int_{-x}^{x} du/(u^2 + 10^{-10})$$

benefits miraculously from the foregoing substitution when $\lambda = 0$ and $\mu = 10^{-5}$, but values near those do almost as well.

Another technique might be called "subdivide and conquer." It subdivides the range of integration into subintervals upon each of which the integrand f(u) is tame, although f(u) may look wild on the range as a whole. For example, $f(u) \equiv \sqrt{u^2 + 10^{-10}}$ has a V-shaped graph practically the same as that of $|u|$. Evaluating $\int_{-3}^{5} f(u)\, du$ accurately takes a long time if done with one press of $\int_y^x$, but subdividing the integral into

$$\int_{-3}^{0} f(u)\, du + \int_0^5 f(u)du$$

takes two presses of $\int_y^x$ and one of **Σ+** but much less time.

Subdivide and conquer works best when combined with apt substitutions. For example, if the formulas in Fig. 5 were unavailable how would $F(\infty) = \int_0^\infty du/(1 + u^{64})$ be calculated?

$$F(\infty) = \int_0^1 du/(1 + u^{64}) + \int_1^\infty du/(1 + u^{64}) \quad \text{... subdivided}$$

$$= \int_0^1 du/(1 + u^{64}) + \int_0^1 w^{62}dw/(w^{64} + 1) \quad \text{... } u=1/w$$

$$= \int_0^1 (1 + u^{62})\, du/(1 + u^{64}) \quad \text{... merged via } w=u$$

$$= 1 + \int_0^1 (u^{62}-u^{64})\, du/(1 + u^{64}) \quad \text{... some algebra}$$

$$= 1 + \tfrac{1}{8}\int_0^1 (1-v^{1/4})\, v^{55/8}\, dv/(1 + v^8) \quad \text{... } u=v^{1/8} \text{ to shrink a tail}$$

$$= 1.000401708155 \pm 1.2\times10^{-12}$$

in 10 minutes at **SCI 8**. Thus we have calculated $F(\infty) = (\pi/64)\csc(\pi/64)$ to 13 significant decimals on a ten-significant-decimal calculator.

Oscillatory integrals like $\int_0^1 \cos(\ln u)\, du$ sometimes succumb to stretching substitutions like $u = v^2$ that damp the oscillations, but generally oscillatory integrals cannot be calculated accurately and quickly without sophisticated tricks beyond the scope of an article like this. A simple trick worth trying when the period of oscillation is known in advance is called *folding*, though it is really another instance of subdivide and conquer. Here is a didactic example.

$$I_3 = \int_0^{600\pi} \frac{\sin^2 u}{\sqrt{u}+\sqrt{u+\pi}}\, du = \text{still running after over three hours at SCI 5}$$

$$= \sum_{n=0}^{599} \int_{n\pi}^{n\pi+\pi} \frac{\sin^2 u}{\sqrt{u} + \sqrt{u+\pi}}\, du$$

$$= \sum_{n=0}^{599} \int_0^{\pi} \frac{\sin^2 v}{\sqrt{v+n\pi} + \sqrt{v+n\pi+\pi}}\, dv$$

after being subdivided and with $u = v + n\pi$. Exchanging $\int$ and $\sum$ produces

$$I_3 = \int_0^{\pi} \sin^2 v \cdot \sum_{n=0}^{599} \frac{1}{\sqrt{v+n\pi} + \sqrt{v+n\pi+\pi}}\, dv.$$

At this point a program should be written to calculate the sum, but because the example is didactic the sum collapses to yield

$$I_3 = \int_0^{\pi} \frac{600 \sin^2 v}{\sqrt{v} + \sqrt{v+600\pi}}\, dv = 21.10204 \pm 0.00007$$

in 5 minutes at **SCI 5**.

Now for a final example drawn from life:

$$V = \int_0^\infty \frac{du}{(a^2+u)\sqrt{(a^2+u)\,(b^2+u)\,(c^2+u)}} \quad \text{for } a = 100, b = 2, c = 1.$$

This integral pertains to the electrostatic field about an ellipsoidal body with principal semiaxes a, b, c.[5] The ellipsoid is needle-shaped like an antenna or a probe. The classical approach transforms V into a standard form called an elliptic integral of the second kind and interpolates on two variables in published tables to get a numerical value. The following approach takes less time.

First transform the improper integral ($\int_0^\infty$) into a proper

one by substituting, say, $u = (a^2-c^2)/(1-v^2) - a^2$ to get

$$V = \lambda \int_{\mu}^{1} \sqrt{(1-v^2)/(v^2+\alpha)}\, dv$$

where

$$\lambda = 2/((a^2-c^2)\sqrt{a^2-b^2}) = 2.00060018 \times 10^{-6}$$

$$\mu = c/a = 0.01$$

$$\alpha = (b^2-c^2)/(a^2-b^2) = 3.001200480 \times 10^{-3}$$

Now, as always happens when $a >> b > c$, the integral is nearly improper because α and μ are both so nearly 0. We suppress this near impropriety by finding an integral in closed form that sufficiently resembles the troublesome part of V. One candidate is

$$W=\lambda \int_{\mu}^{1} dv/\sqrt{v^2+\alpha} = \lambda \ln (v+\sqrt{v^2+\alpha}) \Big|_{v=\mu}^{1}$$

$$= \lambda \ln ((1+\sqrt{1+\alpha})/(\mu+\sqrt{\mu^2+\alpha}))$$

$$= 8.40181880708\times10^{-6}$$

Then

$$V = W + \lambda \int_{\mu}^{1} (\sqrt{(1-v^2)/(v^2+\alpha)} - 1/\sqrt{v^2+\alpha})\, dv$$

$$= \lambda \int_{\mu}^{1} \left(\frac{W/\lambda}{1-\mu} - \frac{v^2}{(1+\sqrt{1-v^2})\sqrt{v^2+\alpha}}\right) dv$$

$$= 7.78867525\times10^{-6} \pm 1.3\times10^{-14}$$

after seven minutes at **FIX 8**. Don't worry about $\sqrt{1-v^2}$ as $v \rightarrow 1$ because the figures lost to roundoff are not needed and its infinite derivative doesn't bother the HP-34C.

Conclusion

A powerful mathematical idea has been placed at the disposal of people who will invoke it with fair confidence by pressing a button marked $\int_y^x$ without having to understand any more about its internal workings than most motorists understand about automatic transmissions. Integrals that might previously have challenged the numerical expert and a big computer now merely amuse the scientist or engineer, and tomorrow they will be routine. And now those engineering students who do attend classes in numerical analysis need no longer be expected to memorize the names nor the remainder terms of quadrature formulas but may instead be taught to use integration wisely.

Acknowledgments

Stan Mintz was the first to request an $\int_y^x$ key for the HP-34C. Dennis Harms helped to select the algorithm and microprogrammed it into the calculator. Robert Barkan wrote the Handbook's two chapters on $\int_y^x$. Then Dennis helped to shorten this article. Working with these people has been a pleasure.

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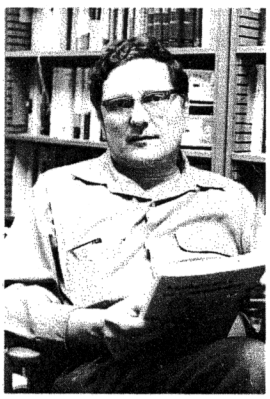

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William Kahan is professor of mathematics and computer science at the University of California at Berkeley. An HP consultant since 1974, he has helped develop increasingly accurate arithmetic and elementary functions for the HP-27, 67/97, 32E, and 34C Calculators and the HP-85 Computer, financial functions for the HP-92 and 38E/C, and other functions for the 32E and 34C, including $\int$ and SOLVE for the 34C. A native of Toronto, Canada, he received his BA and PhD degrees in mathematics and computer science from the University of Toronto in 1954 and 1958, then taught those subjects at Toronto for ten years before moving to Berkeley. A member of the American Mathematical Society, the Association for Computing Machinery, and the Society for Industrial and Applied Mathematics, he has authored several papers and served as a consultant to several companies. He is also co-author of a proposal to standardize binary floating-point arithmetic that has been adopted by several microprocessor manufacturers and is soon to be promulgated by the IEEE. He is married and has two teenage sons.

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AUGUST 1980 Volume 31 • Number 8

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