Title
UCRL LECTURES ON NUMERICAL ANALYSIS AND APPLIED MATHEMATICS, LECTURE III: NUMERICAL INTEGRATION

Author
Baker, James.

Publication Date
1952-10-07

UCRL-2092

UNCLASSIFIED

UNIVERSITY OF CALIFORNIA

Radiation Laboratory

Contract No. W-7405-eng-48

UCRL LECTURES ON NUMERICAL ANALYSIS AND APPLIED MATHEMATICS

Lecture III

James Baker

October 7, 1952

Berkeley, California

DISCLAIMER

UCRL-2092

University of California
Radiation Laboratory
Berkeley, California

UCRL LECTURES ON NUMERICAL ANALYSIS AND APPLIED MATHEMATICS

Lecture III

October 7, 1952

James Baker

NUMERICAL INTEGRATION

1. Introduction

We are interested in evaluating objects of the form, $\int_a^b f(x)\,dx$. Such objects are called definite integrals.

In the event that $f(x) \geq 0$ for $a \leq x \leq b$ we may interpret $\int_a^b f(x)\,dx$ as the area enclosed by the curves, $y = 0$, $y = f(x)$, $x = a$, and $x = b$. The concept of the "area" of such an arbitrary configuration in the plane is built up from our intuitional belief that the 'area' of a rectangle, whose sides have lengths a and b, is a x b.

In order to measure the area of an arbitrary figure we cover it with rectangles, add up the areas of the rectangles to obtain a number, and then take the least of all such numbers. This process is exactly the one used in defining $\int_a^b f(x)\,dx$. However, except in the simplest cases, the use of this definition in evaluating an integral would be tedious so we try to devise a better method.

The best method is given by the following

Theorem: If F is such a function that for every x, $a \leq x \leq b$ implies $F'(x) = f(x)$ then $\int_a^b f(x)\, dx = F(b) - F(a)$.

Unfortunately, we are not always able to find such a function; our knowledge of f may be incomplete; there may be no function F, such that $F' = f$; or we may not be skillful enough or patient enough to find one.

For this reason it becomes necessary to devise other methods for evaluating definite integrals.

2. Motivation

In all that follows, we will be attempting to evaluate $\int_a^b f(x)\, dx$. At this stage of the game we assume f to be continuous in the closed interval $[a, b]$.

What we propose is to replace f in the interval $[a, b]$ by functions whose integral may be evaluated by the fundamental theorem. For example, if we replace f in $[a, b]$ by the function T where

$$T(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a)$$

we obtain

$$\int_a^b T(x)\, dx = \frac{(b - a)}{2}\left[f(a) + f(b)\right]$$

which is the well known trapezoid rule.

In this case we have replaced the function f in the interval $[a, b]$ by the straight line connecting $(a, f(a))$ and $(b, f(b))$, and approximated the integral of f by the integral of the line. The accuracy of this approximation depends, of course, on the character of f in $[a, b]$;

for example, if $a = -1$, $b = +1$, $f(x) = x^2$, then

$T(x) = 1$ and

$$\int_a^b f(x)\,dx = 2/3 \quad \text{while}$$

$$\int_a^b T(x)\,dx = 2 .$$

We can make a better approximation to the integral of f by dividing $[a, b]$ into subintervals and taking the sum of the integrals of the approximating function in each of them. For instance, in the example above, if we divide $[-1, +1]$ into $[-1, 0]$ and $[0, 1]$ we then obtain the following approximation to the integral of f:

$$T(x) = \begin{cases} -x & \text{for } x \in [-1, 0] \\ x & \text{for } x \in [0, 1] \end{cases}$$

$$\int_{-1}^{1} T(x)\,dx = \int_{-1}^{0} x\,dx + \int_{0}^{1} x\,dx = 1 .$$

Thus, we see that the error in the case of one subinterval is $4/3$, while the error in the case of 2 subintervals is $1/3$, and, in fact, the error if we take 2^n subintervals is $4/3.4^n$ which converges rapidly to zero.

It is no coincidence that the values of the integrals of the approximating functions in the above example converge to the integral of f. This happy eventwill occur for every continuous function, using any of the approximating functions which we are about to discuss.

3. Notation

f is a continuous function defined in the closed interval $[a, b]$.

$$h_n = \frac{b-a}{n}$$

$$x_{ni} = a + i\,h_n$$

$$f_{ni} = f(x_{ni})$$

$$I = \int_a^b f(x)\,dx$$

$$T_n = \frac{h_n}{2}\left(f_{no} + 2 f_{n1} + 2 f_{n2} + \cdots + 2 f_{n(n-1)} + f_{nn}\right).$$

If n is even

$$S_n = \frac{h_n}{3}\left(f_{no} + 4 f_{n1} + 2 f_{n2} + 4 f_{n3} + \cdots + 2 f_{n(n-2)} + 4 f_{n(n-1)} + f_{nn}\right).$$

If $[a, b]$ is divided into n equal subintervals, then h_n is the length of each of them; x_{ni} is the coordinate of the i'th division point; and f_{ni} is the function value at the i'th division point. T_n is the quantity obtained by taking the sum of the integrals over $x_{ni}, x_{n(i+1)}$ of the linear functions connecting (x_{ni}, f_{ni}) and $(x_{n(i+1)}, f_{n(i+1)})$. S_n is the quantity obtained by taking the sum of the integrals over $x_{n\,2i}, x_{n\,2(i+1)}$ of the quadratic functions passing through $(x_{n\,2i}, f_{n\,2i})$, $(x_{n(2i+1)}, f_{n(2i+1)})$, and $(x_{n\,2(i+1)}, f_{n\,2(i+1)})$.

The formula used in obtaining T_n is called the trapezoidal rule, and the formula used in obtaining S_n is called Simpson's rule.

4. Techniques

We have listed just two formulas for approximate integration. One can obtain additional formulas by integrating the polynomial of n'th degree which passes through (n + 1) points on the graph of the function. The only advantage of using such formulas is that sometimes by using them one can obtain a given approximation to I with a smaller value of n than would have been needed with the two given formulas.

We have already observed that

$$\lim_{n \to \infty} T_n = I .$$

It is also true that $\lim_{n \to \infty} S_n = I$.

It is now our problem to determine $I - S_n$ for a given n.

In the event that we have a good deal of information about the function f, the following theorem is very useful.

Theorem:

If f is continuous with its first four derivatives in $[a, b]$ then there exists ξ, $a < \xi < b$, such that

$$I - S_2 = -\frac{h_2^5}{90} f^{iv}(\xi) .$$

An obvious corrollary of this theorem, if f satisfies the same hypotheses, is that there exist ξ, $a < \xi < b$ such that

$$E_n = \left| I - S_n \right| \leq \left| \frac{n h_n^5}{180} f^{(iv)}(\xi) \right| .$$

This corollary gives a poorer bound on E_n than that obtained by summing up the results of the theorem on pairs of intervals.

Example:

Let $f(x) = \frac{1}{x}$, $a = 1$, $b = 2$, then

$$I = \int_a^b f(x)\,dx = \ln 2 = .69315 .$$

Let us first consider S_2 .

$x_{2o} = 1$, $x_{21} = \frac{3}{2}$, $x_{22} = 2$

$h = \frac{1}{2}$

$f_{2o} = 1$, $f_{21} = \frac{2}{3}$, $f_{22} = \frac{1}{2}$

$$S_2 = \frac{1}{6}\left(1 + 4\cdot\frac{2}{3} + \frac{1}{2}\right) = .69444 ,$$

hence $E_2 = \left| I - S_2 \right| = .00129$.

Now $f^{(iv)}(x) = \frac{24}{x^5}$ and for $1 \leq \xi \leq 2$

$$\left| f^{(iv)}(\xi) \right| \leq 24$$

so by our theorem

$$E_2 \leq \frac{h_2^5}{90} \left| f^{(iv)}(\xi) \right| \leq \frac{1}{2^5\cdot 90}\cdot 24 = .00833 .$$

Thus we obtain a bound on E_2 which differs from E_2 by a factor of 8 .

Now let us consider S_4 .

$h_4 = \frac{1}{4}$

$x_{4o} = 1$, $x_{41} = \frac{5}{4}$, $x_{42} = \frac{6}{4}$, $x_{43} = \frac{7}{4}$, $x_{44} = 2$

$f_{4o} = 1$, $f_{41} = \frac{4}{5}$, $f_{42} = \frac{4}{6}$, $f_{43} = \frac{4}{7}$, $f_{44} = \frac{1}{2}$

$$S_4 = \frac{1}{12}\left(1 + 4\cdot\frac{4}{5} + 2\cdot\frac{4}{6} + 4\cdot\frac{4}{7} + \frac{1}{2}\right)$$

$$= .69325 \quad .$$

So $\quad E_4 = .00010$

By the corollary we obtain

$$E_4 \leq \frac{4}{4^5 \cdot 180} \left| f^{(iv)}(\xi) \right| \qquad (1 \leq \xi \leq 2)$$

$$\leq \frac{4 \cdot 24}{4^5 \cdot 180} = .00052 \; ,$$

and by the theorem itself

$$E_4 \leq \frac{1}{4^5 \cdot 90} \left(\left| f^{(iv)}(\xi) \right| + \left| f^{(iv)}(\eta) \right| \right) \quad \begin{pmatrix} 1 \leq \xi \leq \frac{3}{2} \\ \frac{3}{2} \leq \eta \leq 2 \end{pmatrix}$$

$$\leq \frac{1}{4^5 \cdot 90} (24 + 4.74074) = .00031$$

So the corollary yields a bound that is five times greater than E_4 , while the bound derived from the theorem differs from E_4 by a factor of 3.

Suppose now that we wish to obtain a result which is correct to five figures. What value should we choose for n? We determine this value by solving the following inequality derived from the corollary:

$$.000005 = 5 \times 10^{-6} \geq E_n$$

$$E_n \leq \frac{n\, h_n^5}{180} \left| f^{(iv)}(\xi) \right| \leq 5 \times 10^{-6}$$

now

$$h_n = \frac{(b - a)}{n} \qquad \text{and} \qquad \left| f^{iv}(\xi) \right| \leq 24 \; , \qquad 1 \leq \xi \leq 2$$

and $b - a = 1$.

So we wish to find n such that

$$\frac{1^5}{n^4(180)} \cdot 24 \leq 5 \times 10^{-6} .$$

Such an n is given by

$$n \geq 10(8/3)^{\frac{1}{4}} = 10 \times 1.28$$

so we should pick $n > 13$.

For $n = 16$ we obtain

$$S_{16} = .6931475$$

but $I = .6931472$

so $E_{16} = 3 \times 10^{-7}$, a considerable improvement on our expectations.

In the event that we are unable to place a bound on the fourth derivative of f it becomes more difficult to place an accurate bound on E_n. We are forced to approximate the fourth derivative by finite differences of the f_{ni}'s. An expression for the error in these terms is given by:

$$E_n \leq \left| \frac{h_n}{90} \left[f_{n(-1)} + f_{n(n+1)} - 4(f_{no} + f_{nn}) + 7(f_{n1} + f_{n(n-1)}) - 8(f_{n2} + f_{n4} + \cdots + f_{n(n-2)}) + 8(f_{n3} + f_{n5} + \cdots + f_{n(n-3)}) \right] \right| \quad \text{for} \quad n \geq 6$$

$$E_2 \leq \left| \frac{h_2}{90} \left[f_{2(-1)} + f_{23} - 4(f_{2o} + f_{22}) + 6 f_1 \right] \right|$$

$$E_4 \leq \left| \frac{h_4}{90} \left[f_{4(-1)} + f_{45} - 4(f_{4o} + f_{44}) + 7(f_{41} + f_{43}) - 8 f_{42} \right] \right| .$$

We note that these formulas involve function values outside of $\left[a, b \right]$.

Let us use this method to place a bound on E_4 for our previous example. Recall that $f(x) = \frac{1}{x}$, $a = 1$, $b = 2$. Now

$$x_{4(-1)} = \frac{3}{4}, \quad x_{45} = \frac{9}{4}, \quad f_{4(-1)} = \frac{4}{3}, \quad f_{45} = \frac{4}{9}$$

$$E_4 \leq \left| \frac{1}{4 \cdot 90} \left[\frac{4}{3} + \frac{4}{9} - 4(1 + 2) + 7\left(\frac{4}{5} + \frac{4}{7}\right) - 8 \cdot \frac{4}{6} \right] \right|$$

$$E_4 \leq .01654$$

Recall that $E_4 = .00010$, the corollary gives $E_4 \leq .00052$, and the theorem gives $E_4 \leq .00031$. So our new bound differs from the actual error by a factor of 100.

Despite this reassuring (if inaccurate) result we are unable to say that this formula will even furnish us with a bound in every case. For example, if we try to evaluate $\int_0^{2\pi} \left| \sin x \right| dx$, and pick $n = 2$, then

$f_{2(-1)} = f_{2o} = f_{21} = f_{22} = f_{23} = 0$, $S_2 = 0$, and our formula in terms of the f_{2i}'s gives us $E_2 \leq 0$, but $E_2 = 4$. So this formula gives us a reasonable bound only if the smoothest curve drawn through (x_{ni}, f_{ni}) does not stray too far from the graph of f.

A more certain (though more laborious) method of checking accuracy is to compute S_n and then compute S_{2n}. If $\left| S_n - S_{2n} \right|$ is smaller than the allowable error it is usually safe to stop. If the difference is greater than the allowable error S_{4n} should be computed and the whole procedure repeated. In our example

$$\left| S_2 - S_4 \right| = .00119, \text{ and } E_4 = .00010.$$

An error of $\mathcal{E}$ in the values of the f_{ni}'s will contribute an error of $(b - a)\cdot\mathcal{E}$ to S_n. For example, if we are integrating over an interval of length ten and wish four figure accuracy, we should compute the f_{ni}'s accurately to five figures.

5. Improper Integrals

If a is not in the domain of f we may still be interested in finding the value of $\int_a^b f(x)\,dx$.

In such cases the most important thing to do is to determine whether the integral exists or not. To investigate the existence of the integral we make the following

Definition: f is of order α at a if there exists $\delta > a$ such that for $a < x < \delta$,

$$f(x) = \frac{\phi(x)}{(a - x)^{\alpha}} \quad \text{where} \quad 0 < \left| \lim_{x \to a} \phi(x) \right| < \infty$$

and state the following.

Theorem: $\int_a^b f(x)\,dx$ exists if and only if f is of order less than one at a.

The above theorem is not as workable as the following one.

Theorem: If $\int_a^b g(x)\,dx$ exists and if for each x in some neighborhood to the right of a $\left| f(x) \right| \leq \left| g(x) \right|$ then $\int_a^b f(x)\,dx$ exists.

For example, let $a = 0$, $b = \frac{\pi}{2}$, $f(x) = \frac{1}{\sqrt{\sin x}}$

$g(x) = \frac{1}{\sqrt{\frac{x}{2}}}$ now for $0 < x < \frac{\pi}{4}$, $\frac{1}{\sqrt{\frac{x}{2}}} \geq \frac{1}{\sqrt{\sin x}}$, i.e., $g(x) \geq f(x)$.

Now $\int_0^{\pi} g(x)\,dx$ exists (since $g(x)$ is of order $\frac{1}{2}$ at 0) hence, $\int_0^{\pi} f(x)dx$ exists.

We call the function g of the above example a **majorant** of the function f. When we have ascertained that $\int_a^b f(x)\,dx$ exists we procede to evaluate it by means of the following

<u>Theorem:</u> If g is a majorant of f in the interval $[a, b]$, then

$$\int_a^b f(x)\,dx \leq \int_a^b g(x)\,dx \; .$$

If f is undefined at a, and g is a majorant of f in some neighborhood to the right of a, and the integral of g over that neighborhood exists, then, if we wish to evaluate $\int_a^b f(x)dx$ with an error of $\mathcal{E}$, we find a number α such that $\int_a^{\alpha} g(x)\,dx < \mathcal{E}$. We then approximate $\int_a^b f(x)dx$ by $\int_{\alpha}^b f(x)\,dx$ which we evaluate by the usual numerical methods.

In the preceding example where $a = 0$, $b = \frac{\pi}{2}$,

$f(x) = \frac{1}{\sqrt{\sin x}}$, and $g(x) = \frac{1}{\sqrt{x/2}}$, suppose we wish to evaluate the integral of f with an error less than $\mathcal{E} = .001$, then α must be such that

$$\mathcal{E} = .001 > \int_0^{\alpha} \frac{1}{\sqrt{x/2}}\,dx = 2\sqrt{2}\,\alpha^{\frac{1}{2}}$$

or

$$\alpha < \frac{10^{-6}}{8}$$

so we might choose $\alpha = 10^{-5}$.

Now $\left| \int_0^{\pi/2} \frac{1}{\sqrt{\sin x}} - \int_{10^{-5}}^{\pi/2} \frac{1}{\sqrt{\sin x}} \right| < .001$, and we may procede, using Simpson's rule or any other method that suits us, to evaluate the latter integral.

Methods for evaluating $\int_a^{\infty} f(x)\, dx$ are very similar to the ones just described. $\int_a^{\infty} f(x)\, dx$ exists if f is of order greater than or equal to one in some neighborhood of infinity, or if there exists g such that for some M, $\int_M^{\infty} g(x)\, dx$ exists and for every $x \geq M$ $\left| g(x) \right| \geq \left| f(x) \right|$.

In order to evaluate $\int_a^{\infty} f(x)\, dx$ within ε we find a majorant, g, of f and an M such that

$$\left| \int_M^{\infty} g(x)\, dx \right| < \varepsilon .$$

We then approximate $\int_a^{\infty} f(x)\, dx$ by $\int_a^{M} f(x)\, dx$ which we evaluate by the usual numerical methods.

6. Integrals in the Plane.

We now wish to study the evaluation of $\int_R f(x, y)\, dA$ where R is a rectangular region in the plane bounded by $x = a$, $x = b$, $y = c$, and $y = d$. We first replace the integral in the plane by the iterated integral $\int_c^d \int_a^b f(x, y)\, dx\, dy$ and let $g(y) = \int_a^b f(x, y)\, dx$. We can then evaluate $g(y_o)$, $g(y_1)$, ... $g(y_n)$ by using Simpson's rule, and then by using Simpson's rule, together with the values we have just determined, evaluate

$$\int_c^d g(y)\, dy = \int_c^d \int_a^b f(x, y)\, dx\, dy = \int_R f(x, y)\, dA .$$

If our original region of integration, say D , is not a rectangle, we may replace D by a rectangle, R , and f by f_1 such that

i) $R \supset D$

ii) $$f_1(x, y) = \begin{cases} f(x, y) & \text{for } (x, y) \in D \\ 0 & \text{for } (x, y) \in R \sim D \end{cases}$$

then

$$\int_D f(x, y)\, dA = \int_R f_1(x, y) dA$$ and we are back to our original case.

To evaluate integrals over spaces of dimension greater than two we follow a procedure exactly analogous to the one outlined above.

7. Bibliography

7.1 Whittaker and Robinson, "Calculus of Observations".

7.2 Milne-Thompson and Comrie, "Standard Four Figure Mathematical Tables", pp. 224 - 225.