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INTEGRATION - ANALYTICAL AND NUMERICAL

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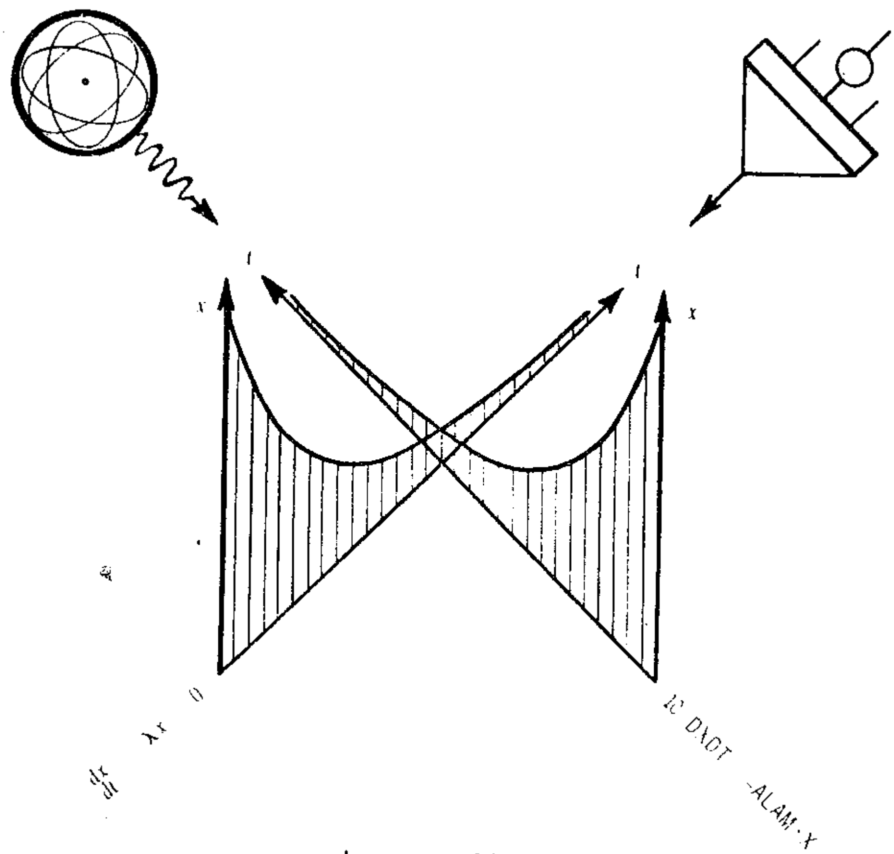
Lecture by B.E. CLANCY



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ABSTRACT

Some numerical methods of evaluating definite integrals are introduced.

CONTENTS

1. INTRODUCTION

The concept of integration is usually introduced - and rightly so - by way of the problem of finding 'the area under a curve'. We are exposed to a diagram such as that in Figure 1 with the curve described by the equation $y = f(x)$ and we learn that the shaded region has area

$$S = \int_a^b f(x)\,dx \quad .$$

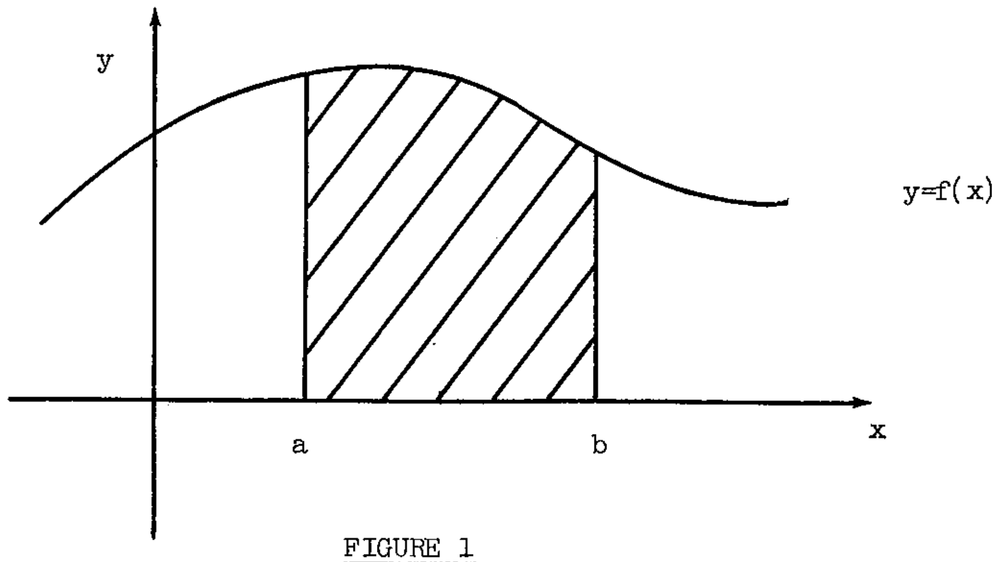

FIGURE 1

There can be no quarrel with this presentation because all integrals can be thought of in these terms.

It was certainly my own experience (and it may be yours too) that this first exposure was followed by a good deal of practice devoted to acquiring skills in tricks for calculating integrals by expressing the answer in terms of formulae and then looking up tables to evaluate the formulae.

To evaluate an integral using a computer it is necessary to learn a new set of tricks - but all of them are based on the idea of an integral being the area under a curve.

2. THE TRAPEZOIDAL RULE

The simplest numerical integration procedure to understand - and one of the easiest to implement - is the trapezoidal rule. If, as in Figure 2, we suppose the segment (a,b) of our original figure divided into 3 equal parts, draw verticals from the subdividing points up to our curve

$y=f(x)$ and join the points of intersection with short straight lines, it is clear that a reasonable approximation to the shaded area in Figure 1 is obtained by calculating the areas of the 3 trapeziums and adding them together.

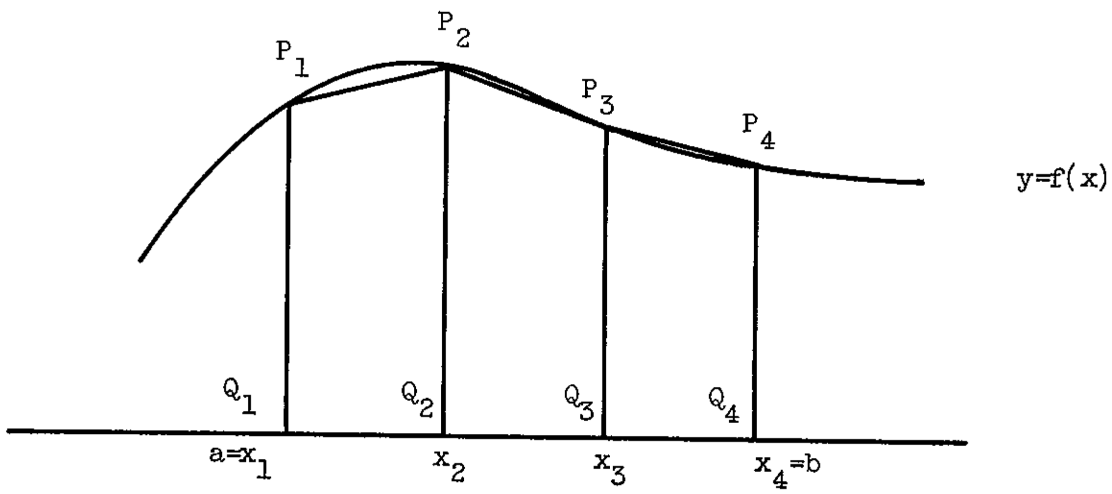

FIGURE 2

Calculation of the individual areas is a straightforward task. The lines $Q_1 P_1$ and $Q_2 P_2$ are of lengths $f(x_1)$ and $f(x_2)$ respectively while the base $Q_1 Q_2$ has length $(b-a)/3$. The area of $Q_1P_1P_2Q_2$ is thus simply

$$\frac{1}{2}\ (f(x_1) + f(x_2)) .\ \frac{b-a}{3}$$

and our approximation to the integral is

$$S \approx \frac{b-a}{6}\left[f(x_1) + 2f(x_2) + 2f(x_3) + f(x_4)\right]$$

That this simple expression should approximate the integral follows from the fact that the sequence of straight line segments $P_1 P_2$, $P_2 P_3$, $P_3 P_4$ follows the curve $y = f(x)$ fairly closely. We can improve our approximation by using more than three subdivisions so that the corresponding sequence of straight line segments together approximate the shape of the curve $y = f(x)$ more closely. If we divide the distance (a,b) into N equal subdivision by points $x_1, x_2, x_3, \ldots, x_{N+1}$ with $x_1=a$ and $x_{N+1}=b$ and with each pair of points a distance $(b-a)/N$ apart, our approximation for the integral becomes

$$S \approx \frac{(b-a)}{2N} \left[f(x_1) + 2\sum_{i=2}^{N} f(x_i) + f(x_{N+1}) \right]$$

For a sufficiently accurate answer we must choose N large enough. A typical procedure for finding out whether or not a large enough value of N has been used is to repeat the calculation using 2N subdivisions and to see whether or not the new answer differs significantly from the old.

It may be interesting to see how the trapezoidal rule tends to get closer to the correct answer as N increases. Let us therefore consider the case where $f(x) = x^2$ and the integral

$$S = \int_0^1 x^2 \, dx = \frac{1}{3} x^3 \Big|_0^1 = \frac{1}{3} .$$

The trapezoidal rule gives, since $f(x_i) = x_i^2 = \left(\frac{i-1}{N}\right)^2$,

$$S \simeq \frac{1}{2N} \left[0 + 2 \sum_{i=2}^{N} \left(\frac{i-1}{N}\right)^2 + 1 \right]$$

$$= \frac{1}{N^3} \left[1^2 + 2^2 + 3^2 + \ldots . + (N-1)^2 \right] + \frac{1}{2N} .$$

We can show that

$$1^2 + 2^2 + 3^2 + \ldots . \; n^2 = \frac{1}{6} n \, (n+1)(2n+1)$$

so that our approximation is

$$S \approx \frac{1}{N^3} \left[\frac{1}{6} (N-1)(N)(2N-1) \right] + \frac{1}{2N}$$

$$= \frac{1}{3} + \frac{1}{6N^2} .$$

As N grows larger the 'error' $\frac{1}{6N^2}$ becomes smaller and tends to zero as N tends to infinity. Even with N = 10 the error is only ½%.

In practice, of course, the summation is carried out numerically rather than analytically as was possible for our example. However, we do have an interesting converse of the trapezoidal rule for the range (0,1) that

$$\sum_{i=2}^{N} f\left(\frac{i-1}{N}\right) \approx N \int_0^1 f(x)\,dx - \frac{1}{2} f(0) - \frac{1}{2} f(1)$$

which gives us a possible way of approximating the analytic sum of a series (provided that we can do the integrals analytically).

The trapezoidal rule is only one of a set of procedures for performing numerical integrations by repeatedly subdividing the baseline (a,b) and approximating the areas of the small strips. In the trapezoidal rule the curve $y=f(x)$ is approximated by small straight line segments. In the second procedure of the set, pairs of strips are used (so that N must be even) and the curve $y=f(x)$ is approximated by a parabola $y=\alpha x^2+\beta x+\gamma$ with coefficients α,β,γ chosen so that the parabola and the curve $y=f(x)$ intersect at the top corners of the strips. This procedure, called Simpson's rule, leads to an approximation of the form

$$S \approx \frac{b-a}{6M} \left\{ f(x_1)+4f(x_2)+2f(x_3)+4f(x_4)+2f(x_5)+ \ldots\ldots \right.$$
$$\left. \ldots +2f(x_{2M-1})+4f(x_{2M})+f(x_{2M+1}) \right\}$$

An approximation using a particular value for N=2M could be improved by doubling N and M and comparing the new answer with the old.

More sophisticated rules have been constructed in which the true curve is fitted by higher order polynomial expressions but these tend not to be used in computing applications.

3. QUADRATURE RULES

Both the trapezoidal rule and Simpson's rule involve the evaluation of the function f(x) at a sequence of points in the interval (a,b), multiplication of the function values by numbers from another sequence and addition of the products to give an approximation to the integral.

They are all of the form

$$S \approx \sum_{i=1}^{L} w_i f(x_i)$$

with the points x_i equally spaced. This general form is sometimes called a quadrature formula.

If the requirement that the points be equally spaced is abandoned and instead the ordinates x_i, the weights w_i and their number L are chosen so that a function f(x) of a particular type will be integrated exactly the quadrature formula is said to be of a Gaussian type.

For L=2 any polynomial of order less than or equal to 3 can be integrated exactly over the interval (a,b) if we choose

$$x_1 = \frac{b}{2}\left(1 - \frac{1}{\sqrt{3}}\right) + \frac{a}{2}\left(1 + \frac{1}{\sqrt{3}}\right) \qquad w_1 = \frac{1}{2}(b-a)$$

$$x_2 = \frac{b}{2}\left(1 + \frac{1}{\sqrt{3}}\right) + \frac{a}{2}\left(1 - \frac{1}{\sqrt{3}}\right) \qquad w_2 = \frac{1}{2}(b-a)$$

With a = -1, b = +1 these become

$$x_1 = -\frac{1}{\sqrt{3}} \qquad w_1 = 1$$

$$x_2 = +\frac{1}{\sqrt{3}} \qquad w_2 = 1$$

and any integral of the form

$$\int_{-1}^{1} (p+qx+rx^2+sx^3)\,dx$$

will be calculated exactly by use of the formula, which is called the Gauss-Legendre formula of order 2.

For L = 3 any polynomial up to fifth order is calculated exactly for the interval (-1, 1) by using

$$x_1 = -\sqrt{\frac{3}{5}} \qquad w_1 = \frac{5}{9}$$

$$x_2 = 0 \qquad w_2 = \frac{8}{9}$$

$$x_3 \quad +\sqrt{\frac{3}{5}} \qquad w_3 = \frac{5}{9}$$

Reference books on numerical analysis list tables of weights and ordinates for Gauss-Legendre formulae of orders up to 96. In many computer applications 16 would be the maximum order used with which polynomials of order up to 33 would be integrated exactly. For integrating functions which are not polynomials, the Gauss-Legendre formulae are used on the basis that a high order polynomial will approximate most functions quite well. The reference books also give tables for the exact integration of integrals of the form

$$\int_{-1}^{1} \frac{(\text{polynomial in } x)}{\sqrt{(1-x^2)}}\, dx \qquad \text{Gauss-Chebyshev}$$

$$\int_{0}^{\infty} e^{-x}.(\text{polynomial in } x)\, dx \qquad \text{Gauss-Laguerre}$$

and for a number of others.

4. THE MONTE CARLO METHOD

This technique is rarely used for simple integrals of the type we have been examining, but it does have application to multiple integrals like

$$\int_{a}^{b} \left[\int_{u(x)}^{v(x)} \left[\int_{p(x,y)}^{q(x,y)} f(x,y,z)\,dz \right] dy \right] dx$$

We will, however, illustrate the method by considering the simple integral

$$\int_{0}^{1} \sqrt{(1-x^2)}\, dx$$

which is just the shaded area in Figure 3.

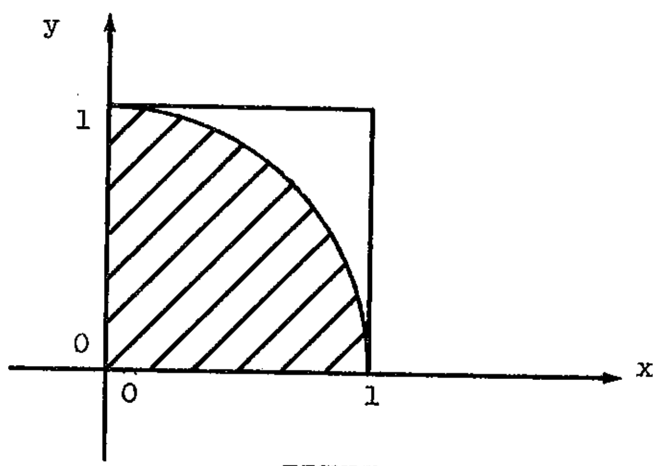

FIGURE 3

The integration techniques we have talked about so far involve the evaluation of the function to be integrated, an evaluation which has to be performed many times. It may happend that this function evaluation is very costly in terms of computer time while at the same time it may be very simple to determine on which side of the curve $y=f(x)$ any given point (x,y) lies. This is almost the case for the example we have chosen. To evaluate $\sqrt{(1-x^2)}$ for a given x takes about 3.6×10^{-4} seconds on the AAEC main computer but given x and y to decide whether or not $x^2 + y^2$ is greater than 1.0 takes about 1.5×10^{-4} seconds. This second test determines whether or not the point x,y lies outside $y = \sqrt{(1-x^2)}$.

We can think of the Monte Carlo procedure as a game of dart playing using Figure 3 as a target. If we assume that the dart player lands his darts uniformly over the outlined square in Figure 3, then the ratio of the number of darts landing in the shaded area to the total number of darts will be approximately the ratio of the area of the shaded figure to the area of the square. In the Monte Carlo procedure we could repeatedly choose a pair of random values for x and y within the square and find out whether or not the point (x,y) is within the circle. Our approximation to the integral would be

$$\frac{\text{Number of hits within circle}}{\text{Number of trials}}$$

5. EXERCISES

When you have completed the exercises set down in the FORTRAN course (AAEC/S1-Pollard) you may care to get more practice by writing a FORTRAN programme to evaluate

$$\int_0^1 \sqrt{(1-x^2)}\,dx$$

using the trapezoidal rule with 100 subdivisions for the interval (0,1).

Then try a programme to do the same integral by the Monte Carlo method using 10000 trials. To get a uniformly distributed random number in the FORTRAN variable X use the statement

```
X = RAND(0)
```

each time a new random value is wanted in the range (0,1).