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Quadrature methods for the evaluation of definite integrals

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QUADRATURE METHODS FOR THE EVALUATION OF DEFINITE INTEGRALS

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QUADRATURE METHODS FOR THE EVALUATION OF DEFINITE INTEGRALS

1. INTRODUCTION

The present Item considers the numerical evaluation of a definite integral of the form

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

where the function $f(x)$ is known analytically.

In cases where the indefinite integral, $\int f(x) \, dx$, can be expressed in terms of well-known simple algebraic or trigonometrical functions, evaluation of the definite integral is straightforward. In other cases it may be difficult or indeed impossible to evaluate an integral by analytical means and for such cases numerical methods are used. The extension of these methods to multiple integrals is also considered.

Frequently the function to be integrated is only specified by a number of discrete values of the function at stations within the range of integration. Such cases usually arise from experimental data and can be treated, for example, by fitting a least-squares curve through the data and integrating the resulting curve. This general topic, and others associated with curve fitting, is not considered in this Item.

Numerous numerical integration formulae have been devised. Those finding most common application are formulae in which the definite integral is expressed solely in terms of the integrand, $f(x)$, at selected values of the variable, x . A common feature of these methods is the essential approximation of the function, $f(x)$, by a polynomial of a certain degree over the range of integration or a part thereof.

Two main classes of formulae worthy of more detailed description are described in the text. The first comprises the Newton-Cotes formulae wherein the selected values of the independent variable are usually chosen to be equally spaced across the integration range. The second class of formulae are termed Gaussian, in which the intervals in x are determined by the condition that the integration formulae have the highest possible degree of accuracy within the limits set by the total number of stations. Selected sources of information supplementary to that in this Item are References 1 to 4 and 6 to 11.

The compromise between effort expended and accuracy of results is of considerable importance and so is discussed in this Item.

A problem that may occasionally arise is that it is desired to integrate up to or across a singularity of the integrand. No general method of coping with this is forthcoming, but some guidance is given in the Item.

Organisations having access to reasonably powerful computation facilities may have ready access to some suitable library programs for evaluating definite integrals. However, to cater for the needs of people not so placed, a computer program is provided and is described in Section 7 of this Item. Examples illustrating the use of the program are given in Section 8.

2. NOTATION

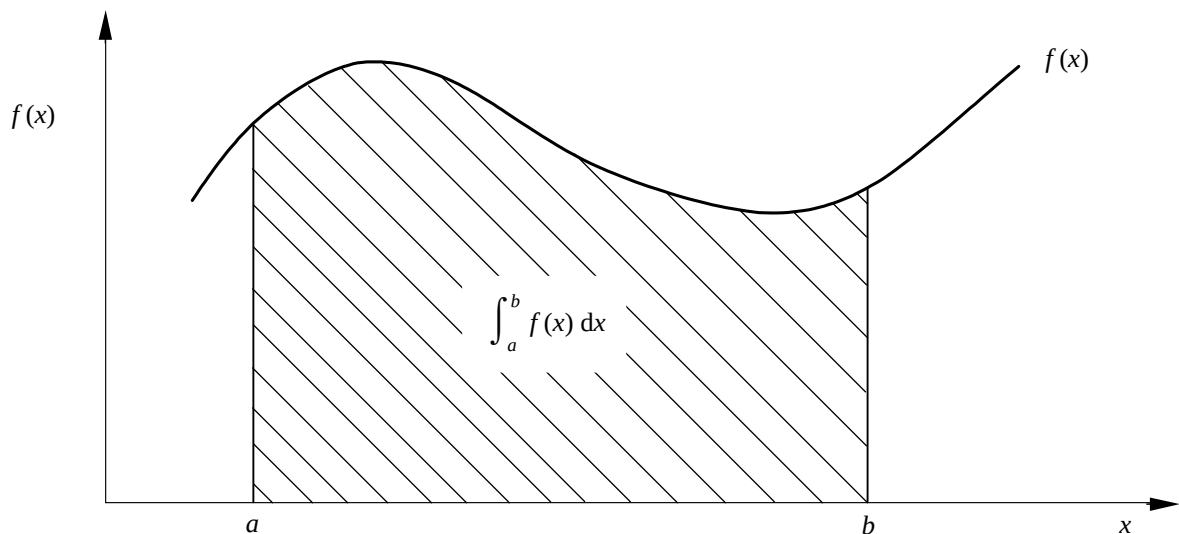
a, b	constant limits of definite single integral or constant outer limits of double integral
$\bar{a}, \bar{b}$	constant limits of part of definite single integral
c, d	constant inner limits of double integral
$c(x), d(x)$	variable inner limits of double integral
$f^{(i)}$	i^{th} derivative of function f
f, g	general functions
$H_n(x)$	n^{th} order Hermite polynomial as function of x
h	step length
i, j, k	variable integers
$L_i(x)$	i^{th} order Lagrangian interpolation polynomial as function of x
$L_n(x)$	n^{th} order Laguerre polynomial as a function of x
l, m, n	general integers
$P_n(x)$	n^{th} order Legendre polynomial as function of x
R_n	remainder or error term used for n^{th} order formula
S	Simpson approximation
w_i	i^{th} weighting factor
x, y, u	independent variables
ε	tolerance of approximation
ξ	general variable

3. QUADRATURE FORMULAE FOR FINITE INTEGRALS

The value of a definite integral of the form,

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

is defined by the geometrical area bounded by the curve $f(x)$, the ordinates at $x = a$ and $x = b$ and the x -axis and is illustrated by the shaded area of Sketch 3.1.



Sketch 3.1 Geometric illustration of single definite integral

Numerical integration or numerical quadrature approximates an integral by a properly weighted sum of the values of the integrand at particular points on the interval of integration. The approximation is of the form

$$\int_a^b f(x) \, dx \approx \sum_{i=0}^n w_i f(x_i), \quad (3.1)$$

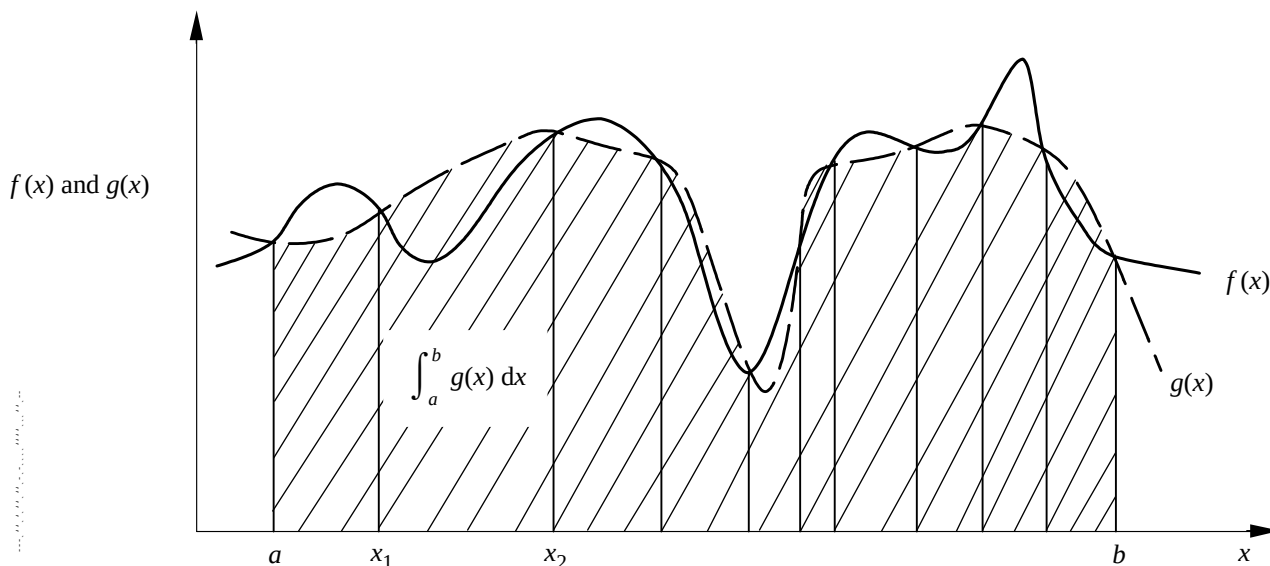
where it is required to specify the abscissae, x_i , and the weights, w_i , such that the right-hand side of Equation (3.1) represents a good approximation to the left-hand side of the equation.

The basis of the approximation of Equation (3.1) is that the function $f(x)$ is replaced by a function $g(x)$ where the functions $f(x)$ and $g(x)$ have identical values at the abscissae points, x_i . The following may then be written

$$\int_a^b f(x) \, dx \approx \int_a^b g(x) \, dx = \sum_{i=0}^n w_i f(x_i), \quad (3.2)$$

in which the w_i values are then evaluated such that the integral involving $g(x)$ is exact. An illustration of $f(x)$ and its approximating function $g(x)$ is given in Sketch 3.2 where the shaded area is the integral of $g(x)$ between $x = a$ and $x = b$.

Any quadrature formulae, of the form of Equation (3.1), should be capable of approximating definite integrals of any function within a margin of error that will diminish, in general, as n is increased. In fact if $f(x)$ is a polynomial of a certain degree then Equation (3.1) can be made exact.



Sketch 3.2 Illustration of $f(x)$ and $g(x)$

Two general approaches are possible when applying the quadrature formula of Equation (3.1) for an integral of a function on the interval (a, b) . Either a single formula may be used over the complete interval or the interval may be subdivided and a single formula used in each subinterval. In the latter case, if it is assumed that the subintervals are equal and that the same formula is used in each, the right-hand side of Equation (3.1) may be re-expressed in a COMPOSITE form as

$$\sum_{i=0}^n w_i f(x_i) = \sum_{j=0}^{m-1} \sum_{k=0}^l w_k f(x_k + jh), \quad (3.3)$$

where m is the number of subintervals, $h = (b - a)/m$ and $(l + 1)$ is the number of points used in each subinterval.

The quadrature formulae in this Item are presented, in general, for integration over a subinterval, or element $(\bar{a}, \bar{b})$, of a complete integration interval (a, b) . The use of such an element recognises the “building-block” approach, where quadrature formulae are usually applied to subintervals of the complete interval (a, b) .

A quadrature formula is defined as one for which the particular choice of the weights and abscissae is such that, when $f(x)$ is a polynomial of order n , the formula is exact. The simplest approach to the choice is to specify evenly-spaced abscissae values along the integration interval (a, b) and choose weight values to give the best approximation. The formulae that result are commonly termed Newton-Cotes formulae and are discussed in Section 3.1. Section 3.2 presents an alternative approach where the abscissae are chosen in such a way that the accuracy is improved.

3.1 Newton-Cotes Formulae

For equally-spaced abscissae values for an element $(\bar{a}, \bar{b})$, Equation (3.1) may be rewritten as

$$\int_{\bar{a}}^{\bar{b}} f(x) \, dx \approx \sum_{i=0}^n w_i f(\bar{a} + ih), \quad (3.4)$$

where the abscissa interval or step length, h , is given by $h = (\bar{b} - \bar{a})/n$.

From Equation (3.4) it can be seen that $(n + 1)$ w_i values are calculated assuming that the approximate function $g(x)$ is a polynomial of order n . When $g(x)$ is any function the terms of which are of the form

$$g(x) = x^j, \quad j = 0, 1, 2, \dots, n$$

and is substituted into Equation (3.4), then the $(n + 1)$ unknown weights can be found from the $(n + 1)$ equations given by

$$\int_{\bar{a}}^{\bar{b}} x^j \, dx = \sum_{i=0}^n w_i (\bar{a} + ih)^j, \quad j = 0, 1, 2, \dots, n. \quad (3.5)$$

An alternative expression for the weights that is easier to solve is

$$w_i = \int_{\bar{a}}^{\bar{b}} L_i(x) \, dx = \int_{\bar{a}}^{\bar{b}} \prod_{\substack{j=0 \\ j \neq i}}^n \frac{(x - x_j)}{(x_i - x_j)} \, dx, \quad (3.6)$$

where $i = 0, 1, 2, \dots, n$ and $L_i(x)$ is the Lagrangian interpolation polynomial corresponding to the abscissae $\bar{a}, \bar{a} + h, \bar{a} + 2h, \dots, \bar{b}$.

The two most frequently used classes of integration formulae are termed CLOSED formulae, which use information about $f(x)$ at both the extreme points, $\bar{a}$ and $\bar{b}$, and OPEN formulae, which do not require information on $f(x)$ at either of these points; for this latter class the weights w_0 and w_n are both zero.

Comparison of the open and closed formulae, which use the same number of computed function evaluations, indicates that the closed formulae are considerably more accurate and so they are almost always used in preference to the open type. For this reason only the Newton-Cotes closed formulae are presented in this Item.

Table 3.1 gives these formulae for n values from 1 to 7 and includes the error or remainder term, R_n , for each formula.

It can be seen from Table 3.1 that the Newton-Cotes formulae of closed type for n values of 1 and 2 are the familiar Trapezoidal and Simpson's Rules respectively, which, it can be noted, may be obtained by approximating the function by fitting a linear function and a quadratic function respectively to the integration interval (a, b) . When the complete integration interval, (a, b) , is segmented into equal subintervals and the same formula is used in each, an Extended or Composite formula is obtained. For the

Trapezoidal Rule the composite formula is found to be

$$\int_a^b f(x) \, dx \approx \frac{h}{2} \left\{ f(x_0) + f(x_n) + 2 \sum_{i=1}^{n-1} f(x_i) \right\}. \quad (3.7)$$

The Extended or Composite Simpson's Rule may similarly be shown to be

$$\int_a^b f(x) \, dx \approx \frac{h}{3} \left\{ f(x_0) + f(x_{2n}) + 4 \sum_{i=1}^{n-1} f(x_{2i-1}) + 2 \sum_{i=1}^{n-1} f(x_{2i}) \right\}, \quad (3.8)$$

where it should be noted that the total abscissa interval has, for notation convenience, been subdivided into $2n$ equal parts, of step length $h = (b - a)/2n$. Similar composite expressions can be derived for any of the Newton-Cotes formulae. The advantage of using a composite formula is that the approximation is continually improved with each successive interval halving and the formula is, consequently, ideally suited to computerisation.

Study of the error term for formulae that use an odd number of function evaluations, say n , and formulae for $(n + 1)$, show that both have the same order of accuracy. Thus the Simpson's rule ($n = 2$) has an accuracy of degree 3. Similarly the Simpson's 3/8 rule ($n = 3$) has the same degree of precision but requires an extra function evaluation. Consequently formulae using an odd number of function evaluations are normally to be preferred.

Considering only the truncation error terms of the formulae, and ignoring rounding error, the use of a high-order formula is, in general, more efficient than the use of a lower-order formula with more subintervals. However, there is a limit to the accuracy achievable, since as the order of formula is increased the higher derivatives of many functions tend to grow rapidly, for example exponential functions, ultimately faster than the powers of h decrease, and so the use of the higher-order formulae is not recommended for general work. Formulae employing more than seven points are rarely used.

Another class of formulae commonly encountered is derived by combining different order Newton-Cotes formulae. Weddle's formula is an example of one of this class that involves the combination of Simpson's rule ($n = 2$) and Simpson's 3/8 rule ($n = 3$). This rule uses seven weighted coefficients and will give exact results if $f(x)$ is a polynomial whose degree does not exceed 5. This is a much lower precision formula than the corresponding formula of Newton-Cotes involving seven functional evaluations ($n = 6$). Weddle's formula has in the past been popular because of the simplicity of its coefficients. Although this formula is not a member of the Newton-Cotes class it has been included for comparison in Table 3.1.

In the quadrature formulae discussed so far, values of the abscissae were chosen at equally spaced intervals. The next section will discuss Gauss-Legendre quadrature, a commonly used class of Gaussian formulae, which places no restriction on the values of the weights or abscissae that are used in Equation (3.1).

TABLE 3.1 Newton-Cotes quadrature formulae (closed type)

$$\int_a^b f(x) \, dx = \sum_{i=0}^n w_i f(a + ih) + R_n$$

$$w_i = \int_a^b L_i(x) \, dx = \int_{x_0}^{x_n} \prod_{\substack{j=0 \\ j \neq i}}^n \frac{(x - x_j)}{(x_i - x_j)} \, dx$$

Name	a	b	n	$\int_a^b f(x) \, dx \approx \sum_{i=0}^n w_i f(x_i)$	R_n
Trapezoidal Rule	x_0	x_1	1	$(h/2)\{f(x_0) + f(x_1)\}$	$-(h^3/12)f^{(2)}(\xi)$ $a \leq \xi \leq b$
Simpson's Rule	x_0	x_2	2	$(h/3)\{f(x_0) + 4f(x_1) + f(x_2)\}$	$-(h^5/90)f^{(4)}(\xi)$ $a \leq \xi \leq b$
Simpson's 3/8	x_0	x_3	3	$(3h/8)\{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\}$	$-(3h^5/80)f^{(4)}(\xi)$ $a \leq \xi \leq b$
Bode's Rule	x_0	x_4	4	$(2h/45)\{7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)\}$	$-(8h^7/945)f^{(6)}(\xi)$ $a \leq \xi \leq b$
---	x_0	x_5	5	$(5h/288)\{19f(x_0) + 75f(x_1) + 50f(x_2) + 50f(x_3) + 75f(x_4) + 19f(x_5)\}$	$-(275h^7/12096)f^{(6)}(\xi)$ $a \leq \xi \leq b$
---	x_0	x_6	6	$(h/140)\{41f(x_0) + 216f(x_1) + 27f(x_2) + 272f(x_3) + 27f(x_4) + 216f(x_5) + 41f(x_6)\}$	$-(9h^9/1400)f^{(8)}(\xi)$ $a \leq \xi \leq b$
---	x_0	x_7	7	$(7h/17280)\{751f(x_0) + 3577f(x_1) + 1323f(x_2) + 2989f(x_3) + 2989f(x_4) + 1323f(x_5) + 3577f(x_6) + 751f(x_7)\}$	$-(8183h^9/518400)f^{(8)}(\xi)$ $a \leq \xi \leq b$

Weddle's Rule	x_0	x_6	5	$(3h/10)\{f(x_0) + 5f(x_1) + f(x_2) + 6f(x_3) + f(x_4) + 5f(x_5) + f(x_6)\}$	—
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3.2 Gauss-Legendre Formulae

The right-hand side of Equation (3.1) contains $(2n + 2)$ unknowns, $(n + 1)$ w_i 's and $(n + 1)$ x_i 's, which is sufficient to specify completely a polynomial of degree $(2n + 1)$. When the approximating polynomial, $g(x)$, is of degree $(2n + 1)$, then the constants, w_i , $i = 1$ to $(n + 1)$ and x_i , $i = 1$ to $(n + 1)$, are uniquely defined.

In a similar manner to the derivation of the Newton-Cotes formulae, $g(x)$ is chosen to be any function the terms of which are of the form

$$g(x) = x^j, \quad j = 0, 1, 2, \dots, 2n + 1,$$

which when substituted into Equation (3.1) gives

$$\int_{\bar{a}}^{\bar{b}} x^j dx = \sum_{i=0}^n w_i x_i^j, \quad j = 0, 1, 2, \dots, 2n + 1. \quad (3.9)$$

Equation (3.9) provides $(2n + 2)$ equations for evaluation of the $(2n + 2)$ w_i and x_i unknowns. Gauss has shown that if the integration interval $(\bar{a}, \bar{b})$ is converted to $(-1, 1)$ by a suitable change of variable, then the x_i 's are roots of the Legendre polynomial of degree $(n + 1)$. Consequently, if the weights are chosen to satisfy Equation (3.9), then Equation (3.9) is exact for polynomials of degree $(2n + 1)$.

Thus the Gauss-Legendre formula of degree n is given by

$$\int_{-1}^1 f(x) dx \approx \sum_{i=0}^{n-1} w_i f(x_i) + R_n, \quad (3.10)$$

where x_i is the i^{th} root of the Legendre polynomial, P_n , of degree n , w_i is the weight at the i^{th} root and R_n is the error term or remainder.

In practice it is not necessary to evaluate the weights and zeros of the Legendre polynomials since they are extensively tabulated in the general literature. However for ease of reference Table 3.2 presents the roots of the Legendre polynomials and the values of the corresponding weights for values of n up to 6.

TABLE 3.2 Gauss-Legendre weights and abscissae

n	x_i	w_i
2	$\pm 1/\sqrt{3}$	1
3	0 $\pm \sqrt{3/5}$	8/9 5/9
4	± 0.86113631 ± 0.33998104	0.3478548451 0.6521451549
5	± 0.90617985 ± 0.53846931 0.0	0.2369268851 0.4786286705 0.5688888889
6	± 0.93246951 ± 0.66120939 ± 0.23861919	0.1713244924 0.3607615730 0.4679139346

The error term or remainder, R_n , of the Gauss-Legendre formulae is given by

$$R_n = \frac{(2)^{2n+1} (n!)^4}{(2n+1)[(2n)!]^3} f^{(2n)}(\xi), \quad -1 \leq \xi \leq 1. \quad (3.11)$$

To convert an integral between limits $(\bar{a}, \bar{b})$ to those required for the Gaussian integration $(-1, 1)$, a linear transformation is used. Thus, for the following integral

$$\int_{\bar{a}}^{\bar{b}} g(u) \, du = \int_{-1}^1 f(x) \, dx,$$

the variable u is mapped by $x = [2u - (\bar{b} + \bar{a})] / (\bar{b} - \bar{a})$, where

$$f(x) = 0.5(\bar{b} - \bar{a}) g\left\{0.5(\bar{b} - \bar{a})x + 0.5(\bar{b} + \bar{a})\right\}.$$

The error terms of these Gaussian formulae involve derivatives of higher-order than the Newton-Cotes formulae and so will suffer even more from truncation error. Consequently only the low-order formulae are normally of practical interest. The Gaussian formulae do have the advantage of high accuracy and provided the magnitudes of the high-order derivatives decrease, or do not increase substantially with increasing n , the Gauss-Legendre formulae can be significantly more accurate than the equal-interval Newton-Cotes formulae for comparable order of n . As was the case for the Newton-Cotes formulae, a composite form of the Gauss-Legendre formulae can be derived for use over the complete integration interval (a, b) . The disadvantages inherent in this procedure are a consequence of the irregular spacing of the abscissae values used in the formulae. Firstly, because the end points of a subinterval are not the values used in the formula, the advantage gained in the Newton-Cotes formulae of having abscissae common to two or more subintervals is not possible. Secondly, a linear transformation of the integration interval is required each time an interval is subdivided and so, although the number of functional evaluations will be smaller for a particular accuracy, the time needed to perform the transformation may well override these advantages.

For satisfactory integration a compromise is consequently needed between the accuracy of the formula, which leads to the use of high-order formulae, and the ease with which a formula can be applied to achieve a specified accuracy, suggesting the use of a low-order composite rule. A better approach, that allows an estimate of the error to be made automatically and distinguishes between the areas in which an accuracy criterion has been met or not met, is called an adaptive procedure and is treated in Section 4.

3.3 Multiple Integrals

All the formulae presented in the earlier parts of this Section 3 may be adapted for the approximation of multiple integrals. The simplest multiple integral is the double integral of the form

$$\int_R \int f(x, y) \, dA.$$

If the region R is rectangular and defined by

$$a \leq x \leq b, \quad c \leq y \leq d,$$

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