FORMULAE FOR NUMERICAL INTEGRATION.

BY W. G. BICKLEY.

Numerical integration, including the numerical integration of differential equations, is becoming increasingly necessary in technical applications. For such purposes, when a very high order of accuracy is not required, formulae which use successive values of the function to be integrated are more convenient than those using differences. Individual authors have given formulae of this type from time to time but a systematic list is not known to the present writer, and would seem to be of service.

The present list gives formulae of four types: (I) formulae for evaluating definite integrals; (II) formulae for forward integration; (III) formulae for integrating over a subrange; and (IV) formulae involving values of both the function and its integral. The leading term in the error series is given. Finally, some comments are made upon the formulae and their uses.

Notation.

The function to be integrated is denoted by $q$, and its integral by $y$, so that, $x$ being the independent variable,

$$q = dy/dx.$$

It is assumed that values of $q$ and $y$ are tabulated (or are being tabulated) at equidistant intervals of $x$; the tabular interval is denoted by $h$. If $x_0$ is a pivotal value of $x$, we denote $q(x_0 + rh)$ by $q_r$, and similarly for $y$. The general form of the formulae given in the first three groups is

$$y_m - y_0 = h \sum_{r=0}^{n} A_r \left(q_r\right).$$

The error term contains a derivative of $q$, and the order of this is indicated by superscript Roman numerals; the argument of this derivative is some value of $x$ between 0 and $mh$.

Group I.

Formulae for evaluating definite integrals.

One-strip.

(I.1)

$$y_1 - y_0 = \frac{h}{2}(q_0 + q_1)$$

[-$q^4h^3/12$

(Trapezoidal rule.)

Two-strip.

(I.2)

$$y_2 - y_0 = \frac{h}{3}(q_0 + 4q_1 + q_2)$$

[-$q^4h^5/90$

(Simpson’s first, or One Third, rule.)
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Three-strip.
(I.3) \( y_3 - y_0 = \frac{3h}{8} (q_0 + 3q_1 + 3q_2 + q_3) \) \[ - 3q^2ih^5/80 \]

(Simpson’s second, or Three Eighths, rule.)

Four-strip.
(I.4) \( y_4 - y_0 = \frac{2h}{45} \{7(q_0 + q_4) + 32(q_1 + q_3) + 12q_2\} \)
\[ - 8q^2ih^7/945 \]

Five-strip.
(I.5) \( y_5 - y_0 = \frac{5h}{288} \{19(q_0 + q_5) + 75(q_1 + q_4) + 50(q_2 + q_3)\} \)
\[ - 275q^2ih^7/12096 \]

Six-strip.
(I.6) \( y_6 - y_0 = \frac{h}{140} \{41(q_0 + q_6) + 216(q_1 + q_5) + 27(q_2 + q_4) + 272q_3\} \)
\[ - 9q^2ih^9/1400 \]

Eight-strip.
(I.8) \( y_8 - y_0 = \frac{4h}{14175} \{989(q_0 + q_8) + 5888(q_1 + q_7) - 928(q_2 + q_6) + 10496(q_3 + q_5) - 4540q_4\} \)
\[ - 2368q^3ih^{11}/467775 \]

Ten-strip.
(I.10) \( y_{10} - y_0 = \frac{5h}{299376} \{16067(q_0 + q_{10}) + 106300(q_1 + q_9) - 48525(q_2 + q_8) + 272400(q_3 + q_7) - 260550(q_4 + q_6) + 427368q_5\} \)
\[ - 134635q^5ih^{13}/326918592 \]

The above are formulae giving the maximum accuracy possible for the number of ordinates used. Other formulae are:

Four-strip.
(I.4a) \( y_4 - y_0 = \frac{h}{3} \{q_0 + q_4 + 4(q_1 + q_3) + 2q_2\} \)
\[ - q^4ih^5/45 \]

(Double Simpson.)

Six-strip.
(I.6a) \( y_6 - y_0 = \frac{3h}{10} \{q_0 + q_6 + 5(q_1 + q_5) + q_2 + q_4 + 6q_3\} \)
\[ - q^6ih^7/140 \]

(Weddle’s rule.)
(I.6b) \[ y_n - y_0 = h \left\{ 0.28 (q_0 + q_6) + 1.62 (q_1 + q_5) + 2.2q_3 \right\} \]
\[ + 9q^6h^7/700 \]
(G. F. Hardy’s rule.)

Ten-strip.
(I.10a) \[ y_{10} - y_0 = \frac{5h}{126} \left\{ 8(q_0 + q_{10}) + 35(q_1 + q_3 + q_7 + q_9) + 15(q_2 + q_4 + q_6) + 36q_5 \right\} \]
\[ - 25q^6h^7/756 \]
(Shovelton’s rule.)

GROUP II.

Formulae for forward integration.

(II.0) \[ y_1 - y_0 = hq_0 \]
\[ + q^2h^2/2 \]

One-strip.
(II.1) \[ y_2 - y_0 = 2hq_1 \]
\[ + q^3h^3/3 \]
(Modified Euler, or Mid-ordinate, rule.)

Two-strip.
(II.2) \[ y_3 - y_0 = \frac{3h}{4}(q_0 + 3q_2) \]
\[ + 3q^4h^4/8 \]
(Heun’s rule.)

Three-strip.
(II.3) \[ y_4 - y_0 = \frac{4h}{3}(2q_1 - q_2 + 2q_3) \]
\[ + 14q^5h^5/45 \]
(Milne’s rule.)

Four-Strip.
(II.4) \[ y_5 - y_0 = \frac{5h}{144}(19q_0 - 10q_1 + 120q_2 - 70q_3 + 85q_4) \]
\[ + 95q^6h^6/288 \]

Five-strip.
(II.5) \[ y_6 - y_0 = \frac{3h}{10}(11q_1 - 14q_2 + 26q_3 - 14q_4 + 11q_5) \]
\[ + 41q^6h^6/140 \]

We may also add:

(II.2a) \[ y_4 - y_0 = \frac{4h}{3}(2q_0 - 4q_1 + 5q_2) \]
\[ + 8q^4h^4/3 \]
GROUP III.

Partial-range formulae.

Two-strip.

\[(\text{III.2}) \quad y_1 - y_0 = \frac{h}{12} (5q_0 + 8q_1 - q_2) \quad [ + q^{iv}h^4/24] \]

Three-strip.

\[(\text{III.3.1}) \quad y_1 - y_0 = \frac{h}{24} (9q_0 + 19q_1 - 5q_2 + q_3) \quad [ - 19q^{iv}h^5/720] \]
\[(\text{III.3.2}) \quad y_2 - y_0 = \frac{h}{3} (q_0 + 4q_1 + q_2) \quad [ - q^{iv}h^5/90] \]

Four-strip.

\[(\text{III.4.1}) \quad y_1 - y_0 = \frac{h}{720} (251q_0 + 646q_1 - 264q_2 + 106q_3 - 19q_4) \quad [ + 3q^{iv}h^6/160] \]
\[(\text{III.4.2}) \quad y_2 - y_0 = \frac{h}{90} (29q_0 + 124q_1 + 24q_2 + 4q_3 - q_4) \quad [ + q^{iv}h^6/90] \]
\[(\text{III.4.3}) \quad y_3 - y_0 = \frac{3h}{80} (9q_0 + 34q_1 + 24q_2 + 14q_3 - q_4) \quad [ + 3q^{iv}h^6/160] \]

Coefficients for five- and six-strip formulae are included in the table given later.

GROUP IV.

Check formulae of high accuracy containing series of values of both \(y\) and \(q\).

Two-strip.

\[(\text{IV.2}) \quad y_2 - y_0 = h (q_0 + 4q_1 + q_2) \quad [ - q^{iv}h^5/90] \]

Three-strip.

\[(\text{IV.3}) \quad 11(y_3 - y_0) + 27(y_2 - y_1) = 3h (q_3 + 9q_2 + 9q_1 + q_0) \quad [ - 3q^{iv}h^7/140] \]

Four-strip.

\[(\text{IV.4}) \quad 25(y_4 - y_0) + 160(y_3 - y_1) \]
\[= 6h \{q_4 + q_0 + 16(q_3 + q_1) + 36q_2\} \quad [ - q^{iv}h^9/105] \]
Six-strip.

(IV.6) \[ 49(y_6 - y_0) + 924(y_5 - y_1) + 2625(y_4 - y_2) \]
\[ = 10h \{q_6 + q_0 + 36(q_5 + q_1) + 225(q_4 + q_2) + 400q_3 \} \]
\[ [ -5q^6 h^{13}/6006 \]

Similar formulae, of lower accuracy, are:

Two-strip.

(IV.2a) \[ y_2 - 2y_1 + y_0 = h(q_2 - q_0)/2 \]
\[ [ -q^{q^6 h^{14}/12} \]

Three-strip.

(IV.3a) \[ 3(y_3 - y_2 - y_1 + y_0) = h(q_3 + 3q_2 - 3q_1 - q_0) \]
\[ [ -q^{q^6 h^{14}/30} \]

Four-strip.

(IV.4a) \[ 11(y_4 + y_0) + 16(y_3 + y_1) - 54y_2 \]
\[ = 3h \{(q_4 - q_0) + 8(q_3 - q_1)\} \]
\[ [ -3q^{q^6 h^{14}/140} \]

Six-strip.

(IV.6a) \[ 137(y_6 + y_0) + 1488(y_5 + y_1) + 375(y_4 + y_2) - 4000y_3 \]
\[ = 30h \{(q_6 - q_0) + 24(q_5 - q_1) + 75(q_4 - q_2)\} \]
\[ [ -5q^{q^6 h^{14}/462} \]

A simple formula of this type is:

(IV.3b) \[ y_3 - y_0 + 9(y_2 - y_1) = 6h(q_2 + q_1) \]
\[ [ +q^{q^6 h^{14}/10} \]

**Remarks on the Formulae.**

**GROUP I.**

The most surprising feature of this group is the fact that the formula for \((2n + 1)\) strips is less accurate than that for \(2n\) strips. This is the explanation of the relatively high accuracy which can, as is well known, be obtained from Simpson’s (first, or one-third) rule. Simpson’s other (three-eighths) rule has a percentage error (for approximately constant \(q^4\)) twice as great. The formulae for seven and nine strips have, in consequence, been omitted.

The presence of negative coefficients (as in the formulae for eight or more strips) is a disadvantage, since this increases the possible rounding-off error.

As the number of strips increases, the coefficients soon become inconvenient. This fact has led to the construction of formulae such as those of G. F. Hardy, Weddle, and Shovelton, in which some accuracy has been sacrificed to obtain simpler coefficients. It may be noted, however, that the errors in the formulae of Hardy and Weddle (both six-strip formulae) are of opposite sign, so that they form a check upon each other, and results are certainly reliable.
as far as they agree. Noting also that the errors are (if powers of \( h \) higher than \( h^2 \) are neglected) in the ratio 9 : −5, it is seen that a combination in the ratio 5 : 9 will be more accurate. Indeed, such a weighted mean is equivalent to the most accurate six-strip rule (I.6).

**Group II.**

This set of formulae is of particular use in the numerical integration of differential equations, since they allow \( y \) to be calculated ahead of the values of \( q \) already tabulated. The error terms given make it possible to form some estimate of the value of \( h \) necessary to secure a desired accuracy. It cannot, however, be too strongly emphasised that these “error” terms cannot give a reliable *a priori* estimate of the resultant error arising in a continuous step-by-step integration—even if an estimate of the appropriate derivative of \( q \) can be found—on account of cumulative error. Thus some independent check at each stage is necessary. The natural check formula is that of group I for the same \( m \) (but see below). In view of the remarks above upon group I, it is advisable that the check formula relate to an even number of strips. The increasing complexity of the coefficients, along with the appearance of negative ones, makes it seldom worth while to use more than four strips, so that the method advocated by Milne, using (II.3) for forward integration, is seen to be probably the best compromise between labour and accuracy.

In connection with Milne’s forward integration formula, there is an advantage in employing first, as a check, the formula

\[
(I.4b) \quad y_4 - y_0 = 2h (q_0 + 4q_2 + q_4) / 3 \quad [ -16q^4h^5 / 45, \\
\]

since the error term is approximately equal to that of the Milne formula \((14q^4h^5 / 45)\) and of opposite sign. If the results disagree only slightly, a simple average may be accurate enough, but it will be found that a combination in the ratio 8 : 7 is equivalent to the most accurate four-strip rule (I.4).

The Heun formula (II.2), although it does not lend itself to the use of an “even” check formula, has nevertheless one great merit. It permits the interval to be halved with facility at any stage. From \( q_{n-2} \) and \( q_n \) we find \( y_{n+1} \), while from \( q_{n-1} \) and \( q_n \) we find \( y_{n+1/2} \), and so obtain three values at interval \( \frac{1}{2}h \).

**Group III.**

In commencing the systematic step-by-step integration of a differential equation, it is evident that the formulae of the preceding groups cannot be applied until a few of the earlier values have been obtained. The method usually advocated is the use of series but this is not always convenient, and in any case needs a subsidiary calculation to determine the necessary coefficients. It is also evident that the accuracy of the whole solution cannot be expected to be greater than that of these early values, upon which everything else
is based. The formulae of group III enable the early values to be obtained by a process of successive approximation, which usually converges rapidly. (If the convergence is not rapid, it is an indication that the interval should be reduced!) Starting with a reasonable approximation to \(q_1\) and \(q_2\) (\(q_0\) being, of course, known) we use (III.2) and (I.2) to obtain approximations to \(y_1\) and \(y_2\). These lead to better approximations to \(q_1\) and \(q_2\), which in their turn lead by the same process to still better ones. We may now start integrating ahead, and return, say by the use of the set (III.4) to improve the accuracy of \(y_1, y_2, y_3\) and \(y_4\).

**Group IV.**

This is a set of formulae of high accuracy, which can be used to supplement other checks, and it is believed that most of them are new. Owing to the small coefficient of the leading \(y\), they are not of much use for integration, because when used to determine this \(y\) rounding-off errors will have considerable effect.

**Derivation.**

A word or two upon the derivation of the formulae may not be out of place. The individual coefficients in groups I-III can be obtained independently as integrals of the appropriate Lagrange interpolation polynomial over the appropriate range. For the calculation of the whole set, however, the use of the Maclaurin series is preferable, since this leads to a set of simultaneous equations for the coefficients which can be solved in a convenient and systematic manner. Also, it is not difficult to show that for constant \(m\), if

\[
y_m - y_0 = \int_0^{mh} q \, dx = h \sum_{r=0}^{n} A_r(n)q_r,
\]

then

(A) \[ A_r^{(n-1)} = A_r^{(n)} - (-1)^{n-r} r! A_{r+1}^{(n)} \]

and

(B) the leading term of the error is \(A_{n+1}^{(n+1)}q^{(n)}h^{n+1}\), unless this vanishes, when we must replace \((n + 1)\) by \((n + 2)\). Finally, we give the formulae of groups I-III, and some additional formulae of these types, in tabular form, classified in a different manner. (A) and (B) are checks on the accuracy of this table, while (B) enables the error term to be obtained in those cases which have not been previously given.

I wish to acknowledge my indebtedness to my colleagues, Messrs. F. J. Turton and G. B. Ehrenborg, who, by drawing my attention to some of these formulae, led me to undertake the systematic investigation whose results are now given.
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TABLE OF COEFFICIENTS

IN THE FORMULA

\[ y_m - y_0 = hN \sum_0^n B_r q_r / D. \]

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1883. She (Countess Benckendorff) was impatient of A. E. Housman’s Cherry Tree poem:

And take from seventy springs a score,
It only leaves me fifty more.

“ I don’t want to do mental arithmetic when I’m reading poetry ” (this though she had a remarkable gift for mathematics). But Bertrand Russell had told me that great mathematicians were usually weak in their sums.—Sir Edward Marsh, Memoirs, Sunday Times, January 8, 1939. [From the Rev. E. M. Radford; Mr. P. J. Harris.]