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SURVEY OF EXTRAPOLATION PROCESSES IN NUMERICAL ANALYSIS*

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Abstract. This survey traces the development of extrapolation processes in numerical analysis, dealing mainly with those based on polynomial or rational functions. The more important results are presented in a uniform notation and interconnections between work in different fields are brought out. An extensive bibliography is appended.

1. Introduction. This survey traces the development of extrapolation processes in numerical analysis, dealing mainly with those based on polynomial or rational functions. An extensive search of the English, German and French mathematical literature was carried out so that individual contributions could be placed in their historical perspective. Many of the earlier works are somewhat obscure and have been overlooked by other reviewers. In this survey the more important results are presented in a uniform notation and interconnections between work in different fields are brought out.

The sections follow each other in roughly chronological order as do the references within each section. Citations of works which deal with extrapolation processes appear in capitals and an author index has been appended for ease of reference. The following abbreviations are used:

BV — Boundary Value,
EV — Eigenvalue,
IV — Initial Value,
IE — Integral Equation,
ODE — Ordinary Differential Equation,
PDE — Partial Differential Equation.

Often in numerical analysis an unknown quantity, a_0, is approximated by a calculable quantity, $T(h)$, depending on a parameter $h > 0$, such that

$$T(0) \equiv \lim_{h \to 0} T(h) = a_0,$$

and it is known that there exist constants $a_1, a_2, \cdots, \gamma_1, \gamma_2, \cdots, C_1, C_2, \cdots$, and H_0 such that, for $J = 1, 2, 3, \cdots$, and $h < H_0$,

$$T(h) = a_0 + a_1 h^{\gamma_1} + a_2 h^{\gamma_2} + \cdots + a_J h^{\gamma_J} + R_J(h), \tag{1}$$

where $|R_J(h)| < C_J h^{\gamma_{J+1}}$ and $0 < \gamma_1 < \gamma_2 < \cdots < \gamma_J < \gamma_{J+1}$.

That is, $T(h)$ "admits an asymptotic expansion for $h \to 0$." We do not assume that the infinite series $a_0 + a_1 h^{\gamma_1} + a_2 h^{\gamma_2} + \cdots$ converges.

In this situation it is natural to attempt to accelerate the convergence of the approximations towards a_0. Ways in which this "extrapolation" (to $h = 0$) can be carried out for a variety of problems are discussed in the following sections.

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2. Approximating π. Archimedes (250 BC) obtained bounds for π by calculating the perimeters of regular polygons inscribing and circumscribing a circle of unit diameter. Using 96-sided polygons he was able to prove that $3\frac{10}{71} < \pi < 3\frac{1}{7}$.

In order to show that his approximations are of form (1), let us denote the perimeter of the n-sided inscribed polygon by T_n, or $T(h)$, where $nh = 1$. It is easily verified that

$$T_n = n \times \sin(\pi/n)$$

or

$$T(h) = (1/h) \times \sin(\pi h).$$

Now

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \cdots + \frac{(-)^j x^{2j+1}}{(2j+1)!} + \cdots$$

(convergent for all x), so

$$T(h) = \frac{1}{h} \times \left(\pi h - \frac{(\pi h)^3}{3!} + \frac{(\pi h)^5}{5!} - \cdots + \frac{(-)^j (\pi h)^{2j+1}}{(2j+1)!} + \cdots \right),$$

or

$$T(h) = \pi - \frac{\pi^3}{3!}h^2 + \frac{\pi^5}{5!}h^4 - \cdots + (-)^j \frac{\pi^{2j+1}}{(2j+1)!}h^{2j} + \cdots, \tag{2}$$

which is of form (1), with

$$a_j = (-)^j(\pi^{2j+1}/(2j+1)!), \qquad j = 0, 1, 2, \cdots,$$

$$\gamma_j = 2j, \qquad j = 1, 2, 3, \cdots.$$

For $h < 1$, $T(h) < \pi$, so $\{T_n\}$ is a sequence of lower bounds for π, increasing with n. Similarly, the perimeter of the n-sided circumscribing polygon is given by:

$$U_n = U(1/n) = n \times \tan(\pi/n).$$

Thus

$$U(h) = \pi + \frac{\pi^3}{3}h^2 + \frac{2\pi^5}{15}h^4 + \frac{17\pi^7}{315}h^6 + \cdots \tag{3}$$

(convergent for $h < \frac{1}{2}$), and $\{U_n\}$ is a decreasing sequence of upper bounds for π. The bounds for $n = 6, 12, 24, 48$ and 96 are shown in Table 1, to 4 decimal places (4D). To this accuracy, Archimedes' bounds are 3.1408 and 3.1429.

TABLE 1

n	6	12	24	48	96
T_n	3.0000	3.1058	3.1326	3.1393	3.1410
U_n	3.4641	3.2154	3.1597	3.1461	3.1427

Subsequent refinements obtained using Archimedes' method are shown in Table 2 (information from Rudio (1892), Moors (1905), Turton (1946), Dijksterhuis (1954), Eves (1969)), where all dates are AD and "accuracy" means number of decimal places correct.

TABLE 2

Name	Aryabhata	Vieta	Romanus	van Ceulen
Date	530	1579	1593	1610
Accuracy	4	9	15	35
n	6×2^6	6×2^{16}	2^{30}	2^{62}

Several attempts had been made to reduce the amount of calculation required to obtain accurate approximations before HUYGENS (1654) suggested using two new sequences, $\{S_n\}$ and $\{V_n\}$, defined by

$$S_n \equiv S(h) \equiv (4T(h) - T(2h))/3 \tag{4}$$

and

$$V_n \equiv V(h) \equiv (2U(h) + T(2h))/3. \tag{5}$$

He used geometric arguments (see Hardingham (1932), Lodge (1935), Whiteside (1960), Hofman (1966)) to show that

$$S_n < \pi < V_n$$

(SNELL (1621) had stated, without proof, that $V_n > \pi$). GREGORY (1667) subsequently proved a similar result for a general central conic.

Expansions (2) and (3) can be used to show that

$$S(h) = ((4 - 1)a_0 + (4 - 2^2)a_1h^2 + (4 - 2^4)a_2h^4 + (4 - 2^6)a_3h^6 + \cdots + (4 - 2^{2j})a_jh^{2j} + \cdots)/3,$$

i.e.

$$S(h) = a_0 - 4a_2h^4 - 20a_3h^6 - \cdots - (4^j - 4)a_jh^{2j}/3 + \cdots = \pi - \frac{\pi^5}{30}h^4 + \frac{\pi^7}{252}h^6 - \cdots, \tag{6}$$

and

$$V(h) = \pi + \frac{2\pi^5}{15}h^4 + \frac{2\pi^7}{63}h^6 + \cdots.$$

The terms in h^2 have been eliminated and the errors in $S(h)$ and $V(h)$ are only $O(h^4)$. Thus $S(1/2^{30})$ is correct to 35D. Formula (4) *accelerates the convergence* of the sequence $\{T_n = T(h)\}$ towards π.

MILNE (1903) extended this idea, showing that the terms in $h^2, h^4, \cdots, h^{2m}$ can be eliminated by solving the system of linear equations

$$\begin{aligned} T(h) &= b_0 + b_1 h^2 + \cdots + b_m h^{2m}, \\ T(h/2) &= b_0 + b_1 (h/2)^2 + \cdots + b_m (h/2)^{2m}, \\ &\cdots \\ T(h/2^m) &= b_0 + b_1 (h/2^m)^2 + \cdots + b_m (h/2^m)^{2m}, \end{aligned} \tag{7}$$

where the b_j are, in some sense, approximations to the a_j. b_0 is an approximation to π (or, more generally, to the length of a circular arc), obtained by combining together the cruder approximations $T(h), T(h/2), \cdots, T(h/2^m)$. If we define

$$T(h, h/2, \cdots, h/2^m) \equiv b_0 \equiv \sum_{k=0}^{m} \alpha_k T(h/2^k) \tag{8}$$

we find that

$$\alpha_k = (-)^{m-k} 2^{k(k+1)} \Big/ \left(\left(\prod_{i=1}^{k} (4^i - 1) \right) \times \left(\prod_{j=1}^{m-k} (4^j - 1) \right) \right).$$

For example,

$$T(h, h/2) = (4T(h/2) - T(h))/3,$$

i.e.,

$$T(h, h/2) \equiv S(h/2). \tag{9}$$

Similarly

$$T(h, h/2, h/4) = (64T(h/4) - 20T(h/2) + T(h))/45. \tag{10}$$

Using $h = \frac{1}{6}$, $m = 4$, π can be computed to 16D.

3. Numerical integration. One class of quadrature rules for approximating

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

uses weighted sums of the values of the integrand at equidistant points

$$x_0 = a, \quad x_1 = a + h, \quad x_2 = a + 2h, \cdots, \quad x_n = a + nh = b.$$

The simplest of these is the *trapezoidal rule*:

$$T(h) \equiv \tfrac{1}{2} h \{ f_0 + 2f_1 + 2f_2 + 2f_3 + 2f_4 + \cdots + 2f_{n-1} + f_n \}, \tag{11}$$

where

$$f_r \equiv f(x_r) = f(a + rh), \qquad r = 0, 1, \cdots, n.$$

When n is even we may use *Simpson's rule*:

$$S(h) \equiv \tfrac{1}{3} h \{ f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + 4f_{n-1} + f_n \}. \tag{12}$$

When n is divisible by 3 ($3|n$), we have *Newton's $\frac{3}{8}$ rule*:

$$N(h) \equiv \tfrac{3}{8}h\{f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + \cdots + 3f_{n-1} + f_n\}, \tag{13}$$

and when $4|n$, *Boole's rule*:

$$B(h) \equiv \tfrac{2}{45}h\{7f_0 + 32f_1 + 12f_2 + 32f_3 + 14f_4 + \cdots + 7f_n\}. \tag{14}$$

These four rules are examples of *composite Newton–Cotes integration formulas*, based on approximating the integrand by a piecewise interpolating polynomial (Davis and Rabinowitz (1967, p. 29)).

Other rules, which do not belong to the Newton–Cotes class of formulas, are *Weddle's rule* (Weddle (1854)):

$$W(h) \equiv \tfrac{3}{10}h\{f_0 + 5f_1 + f_2 + 6f_3 + f_4 + 5f_5 + 2f_6 + \cdots + 5f_{n-1} + f_n\}, \tag{15}$$

and *Hardy's rule* (Hardy (1883)):

$$H(h) \equiv \tfrac{1}{50}h\{14f_0 + 81f_1 + 110f_3 + 81f_5 + 28f_6 + \cdots + 81f_{n-1} + 14f_n\}, \tag{16}$$

which are applicable when $6|n$.

SHEPPARD (1900) observed that these rules can be obtained by linear combination of trapezoidal approximations for different values of h. For instance, Simpson's rule may be obtained by combining $T(h)$ and $T(2h)$, thus:

$$\begin{aligned}(4T(h) - T(2h))/3 &= (4 \times \tfrac{1}{2}h\{f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n\} \\ &\quad - \tfrac{1}{2}(2h)\{f_0 + 2f_2 + \cdots + f_n\})/3 \\ &= \tfrac{1}{3}h(\{2f_0 + 4f_1 + 4f_2 + \cdots + 4f_{n-1} + 2f_n\} \\ &\quad - \{f_0 + 2f_2 + \cdots + f_n\}) \\ &= \tfrac{1}{3}h\{f_0 + 4f_1 + 2f_2 + \cdots + 4f_{n-1} + f_n\}.\end{aligned}$$

So

$$S(h) \equiv (4T(h) - T(2h))/3$$

(compare (4)). He also noted that

$$N(h) \equiv (9T(h) - T(3h))/8$$

and

$$W(h) \equiv (15T(h) - 6T(2h) + T(3h))/10 \tag{17}$$

(HARDY (1883) had observed that $W(h) \equiv (9S(h) - 4N(h))/5$).

To generalize these results he called on the *Euler–Maclaurin summation formula* (Euler (1738), Maclaurin (1742)):

$$\begin{aligned}T(h) = I &+ \frac{B_1}{2!}(f'(b) - f'(a))h^2 - \frac{B_2}{4!}(f'''(b) - f'''(a))h^4 \\ &+ \cdots + (-)^{J-1}\frac{B_J}{(2J)!}(f^{(2J-1)}(b) - f^{(2J-1)}(a))h^{2J} + R_J\end{aligned} \tag{18}$$

where $B_1 = \frac{1}{6}$, $B_2 = \frac{1}{30}$, $B_3 = \frac{1}{42}$, $\cdots$ are the *Bernoulli numbers* (Whittaker and Watson (1927, pp. 125–128), Sheppard (1930), Grant (1969). Another notation, with $B_2 = \frac{1}{6}$, $B_4 = -\frac{1}{30}$, $B_6 = \frac{1}{42}$, $\cdots$ and $B_{2j+1} = 0$ for $j = 1, 2, 3, \cdots$, is used by Jordan (1950, p. 233) and other authors). It is convenient to define

$$\beta_j = B_j/(2j)!. \tag{19}$$

Equation (18) is of the form (1), with

$$T(0) = a_0 = I,$$

and, for $j = 1, 2, 3, \cdots$,

$$a_j = (-)^{j-1}\beta_j(f^{(2j-1)}(b) - f^{(2j-1)}(a)), \qquad \gamma_j = 2j.$$

Thus (as in (6))

$$S(h) = I - 4a_2h^4 - 20a_3h^6 - \cdots - (4^j - 4)a_jh^{2j}/3 - \cdots.$$

Similarly

$$N(h) = I - 9a_2h^4 - 90a_3h^6 - \cdots - (9^j - 9)a_jh^{2j}/8 - \cdots$$

and

$$W(h) = I + 36a_3h^6 + 504a_4h^8 + \cdots + (9^j - 6 \times 4^j + 15)a_jh^{2j}/10 + \cdots.$$

In the last case the terms in h^2 *and* h^4 have been eliminated. Sheppard suggested extending the process by combining $m + 1$ trapezoidal values with different steps to eliminate $h^2, h^4, \cdots, h^{2m}$ and obtain the $O(h^{2m+2})$ approximation

$$T(h_0, h_1, \cdots, h_m) = \sum_{k=0}^{m} \alpha_k T(h_k)$$

(compare (8)), where $h_k = r_kh$, $1 = r_0 < r_1 < \cdots < r_m$, and the α_k depend on the sequence $\{r_k\}$ and satisfy

$$\begin{aligned} \alpha_0 + \alpha_1 + \cdots + \alpha_m &= 1, \\ \alpha_0 r_0^2 + \alpha_1 r_1^2 + \cdots + \alpha_m r_m^2 &= 0, \\ \alpha_0 r_0^4 + \alpha_1 r_1^4 + \cdots + \alpha_m r_m^4 &= 0, \\ &\cdots \\ \alpha_0 r_0^{2m} + \alpha_1 r_1^{2m} + \cdots + \alpha_m r_m^{2m} &= 0. \end{aligned} \tag{20}$$

It can be shown that if we solve (20) with $r_k = 2^{-k}$ we obtain the same expression for α_k as Milne obtained by solving (7). Apart from the choice of r_k, the two approaches are completely equivalent. For example,

$$T(h, 2h) = (4T(h) - T(2h))/3 \equiv S(h) \tag{21}$$

(compare (9)),

$$\begin{aligned} T(h, 3h) &= (9T(h) - T(3h))/8 \equiv N(h), \\ T(h, 2h, 3h) &= (15T(h) - 6T(2h) + T(3h))/10 \equiv W(h), \\ T(h, 2h, 4h) &= (64T(h) - 20T(2h) + T(4h))/45 \end{aligned}$$

(compare (10)). It is easily verified that

$$T(h, 2h, 4h) \equiv B(h). \tag{22}$$

Sheppard also used the following sequences $\{r_k\}$: $\{1, 5\}$, $\{1, 2, 5\}$, $\{1, 3, 5\}$, $\{1, 3, 9\}$, $\{1, 2, 3, 4\}$, $\{1, 2, 3, 6\}$, $\{1, 2, 4, 8\}$, $\{1, 2, 5, 10\}$ and $\{1, 2, 3, 4, 6\}$. He noted that, if $f'(b) = f'(a)$,—i.e., $a_1 = 0$—then $T(h)$ is usually more accurate than $S(h)$, having a smaller coefficient of h^4. In this case we can choose the $\{\alpha_k\}$ to eliminate $h^4, h^6, \cdots, h^{2m+2}$. Similarly, if also $f'''(b) = f'''(a)$, then $T(h)$ is usually more accurate than $W(h)$.

He observed that the *midpoint* or *rectangle rule*,

$$U(h) \equiv h\{f_{1/2} + f_{3/2} + f_{5/2} + \cdots + f_{n-1/2}\}, \tag{23}$$

can be obtained from

$$U(h) = 2T(h/2) - T(h), \tag{24}$$

and hence

$$U(h) = I - \tfrac{1}{2}a_1h^2 - \tfrac{7}{8}a_2h^4 - \cdots - (1 - 2^{1-2j})a_jh^{2j} - \cdots. \tag{25}$$

Thus the same elimination techniques can be applied to $U(h)$. He noted that they are also applicable to *modified* rules like *Parmentier's rule*,

$$P(h) \equiv U(h) + \tfrac{1}{12}h\{f_0 - f_{1/2} - f_{n-1/2} + f_n\} \tag{26}$$

(which has error $O(h^4)$), and to *product* rules for the approximation of

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

BUCHANAN (1902, 1903) used the central difference form of (18) to obtain (20) and noted that

$$T(h, 2h, 3h, 6h) = (9W(h) + 5H(h))/14. \tag{27}$$

It is easily verified that $T(h, 2h, 3h, 6h)$ is the Newton–Cotes 7-point rule.

COREY (1906) suggested eliminating the terms in h^{2q+2}, h^{2q+4}, h^{2q+6}, $\cdots$, h^{2q+2m} from the expansion for the *corrected trapezium rule*,

$$T_q(h) \equiv T(h) - \beta_1(f'(b) - f'(a))h^2 + \beta_2(f'''(b) - f'''(a))h^4 - \cdots + (-)^q\beta_q(f^{(2q-1)}(b) - f^{(2q-1)}(a))h^{2q}$$

(compare (18)), to obtain $T_q(h_0, h_1, \cdots, h_m)$ with error $O(h^{2q+2m+2})$. Obviously $T_0(h) \equiv T(h)$ and

$$T_0(h_0, h_1, \cdots, h_m) \equiv T(h_0, h_1, \cdots, h_m),$$

so this is a generalization of Sheppard's technique, to be used when the values of $f', f''', \cdots, f^{(2q-1)}$ are known at a and b. Corey used $1 \geqq r_0 > r_1 > \cdots > r_m$, and recommended that, in choosing the $\{r_k\}$, we should "take the largest value (of $1/r_k$) such that one or more of the lesser values will be submultiples thereof"—e.g., $\{\frac{1}{2}, \frac{1}{3}, \frac{1}{6}\}$—thus economizing on function evaluations.

BECKER (1911) showed how $U(2h)$ could be combined with the $T(h_k)$, for $k = 1, 2, \cdots, m$, in such a way as to eliminate the terms in $h^2, h^4, \cdots, h^{2m}$ from the error. For example,

$$S(h) = (2U(2h) + T(2h))/3 \tag{28}$$

(see also PIAGGIO (1918, 1920)). Since $U(2h) \equiv 2T(h) - T(2h)$, the resulting methods are identical with Sheppard's. Becker noted that the "semiconvergence" of the Euler–Maclaurin series may limit m, and advised choosing m then h. He made the important point that, although $S(h)$, $N(h)$, $B(h)$ and the Newton–Cotes 7-point rule can be obtained in this fashion, the 9- and 11-point Newton–Cotes formulas cannot.

4. Numerical solution of differential equations. There are many numerical methods which approximate the solution a_0 of a continuous problem (e.g., a differential equation) by applying a "discretization process" with "mesh width" h and obtaining the solution $T(h)$ of the resulting discrete problem (see, e.g., Henrici (1962)). RICHARDSON (1910) observed that the use of central differences in the discretization often leads to errors of the form

$$T(h) - a_0 = a_1h^2 + a_2h^4 + a_3h^6 + \cdots, \tag{29}$$

where $T(0) = a_0$ and the a_j are independent of h. T and the a_j will be vectors if the solution has several components.

Richardson suggested eliminating the term in h^2 by combining the approximations obtained with two different mesh widths, h_0 and h_1:

$$T(h_0, h_1) = \frac{h_1^2T(h_0) - h_0^2T(h_1)}{h_1^2 - h_0^2} \tag{30}$$

(note that, if $h_0 = h$ and $h_1 = 2h$, we obtain (4)). He applied this method, which he called the *deferred approach to the limit*, to:

(a) vibration of a stretched string of beads;

(b) Laplace's equation in a square—in this case $a_0 = \phi(x, y)$, where $\nabla^2\phi \equiv \partial^2\phi/\partial x^2 + \partial^2\phi/\partial y^2 = 0$, T and the a_j $(j > 0)$ will be functions of x and y, and (30) can only be applied if $T(h_0)$ and $T(h_1)$ refer to the same point (x, y);

(c) vibration of a clamped plate;

(d) stresses in a masonry dam.

In (c) he also obtained $T(h_0, h_1, h_2)$ by solving

$$T(h_k) = T(h_0, h_1, h_2) + b_1h_k^2 + b_2h_k^4, \qquad k = 0, 1, 2 \tag{31}$$

(compare (7)).

RUNGE (1912) suggested that $(T(2h) - T(h))/15$ could be used as an estimate of the error in $T(h)$ when solving ordinary differential equations (ODE's) approximately by means of the Runge–Kutta 4th order method (Runge (1895); Kutta (1901)). In this case, if the ODE is $y' = f(x, y)$, we have $a_0 = y(x)$ and $T(h) = a_0 + O(h^4)$.

Later RICHARDSON (1923) used (30) to improve numerical solutions of an integral equation. In another paper, RICHARDSON (1925) noted that at discon-

tinuities the series in (29) may not converge, but commented "there are, so to speak, in the mathematical country, precipices and pit-shafts down which it would be possible to fall, but that need not deter us from walking about."

Subsequently, RICHARDSON (1927) examined the deferred approach to the limit in greater detail, noting in passing that it had also been considered by BOGOLOUBOFF and KRYLOFF (1926). He showed that the method could be applied to:

(a) improve Archimedes' approximations to π (see § 2);
(b) accelerate the convergence of a sequence;
(c) obtain the second moment of grouped data;
(d) compute Fourier coefficients;
(e) solve a 6th order differential eigenvalue problem.

In each case he used pairs of approximations to eliminate h^2 (as in (30)), a process he named "h^2-extrapolation," and in (e) he also combined three approximations in such a way as to eliminate h^2 *and* h^4 (as in (31)), a process we shall name "(h^2, h^4)-extrapolation."

In (b) we have

$$T_n = ((2n + 1)/(2n - 1))^n$$

and we assume that

$$T_n = a_0 + a_1/n + a_2/n^2 + \cdots \tag{32}$$

and

$$\lim_{n\to\infty} T_n = a_0. \tag{33}$$

But

$$T_{-n} = ((-2n + 1)/(-2n - 1))^{-n} = T_n,$$

which implies

$$a_1 = a_3 = \cdots = a_{2j+1} = \cdots = 0,$$

so we have an expansion of form (29) with $T(h) = T_n$ and $nh = 1$.

Richardson went on to:

(a) suggest rules for replacing the continuous problem by a suitable discrete problem (using central differences);

(b) show how the deferred approach to the limit may be affected by the presence of singularities and discontinuities;

(c) derive an admittedly laborious method for estimating how small h should be to make the process valid.

In a companion paper, GAUNT (1927) investigated the numerical solution of an nth order ODE, which can be written as a system of n first order ODE's:

$$\underline{y}' = \underline{f}(x, \underline{y}), \qquad \underline{y}(x_0) = \underline{y}_0, \tag{34}$$

by using the *midpoint method* (or "method of interpenetrating lattices"):

$$\underline{Y}_{r+1} = \underline{Y}_{r-1} + 2h\underline{f}(x_r, \underline{Y}_r), \tag{35}$$

where $\underline{Y}_r = \underline{Y}_r(h)$ is an approximation to the value of $\underline{y}$ at $x = x_r = x_0 + rh$. He concluded that h^2-extrapolation can be applied to $\underline{T}(h_k) = \underline{Y}_{n_k}(h_k)$, where $h_k \to 0$ and $n_k \to \infty$ in such a manner that $n_k h_k$ remains fixed, provided the first step is taken according to a special formula. Taking the exact value—i.e., $\underline{Y}_1 = \underline{y}(x_0 + h)$—usually invalidates the process! He observed that "there would be no essential difficulty in extending the expansion beyond the fourth power of h; but such a refinement would have little practical value."

WILLERS (1928) generalized Runge's error estimate, suggesting $(T(2h) - T(h))/(2^p - 1)$ as an estimate of the error in $T(h)$ when a pth order method is used for solving ODE's.

5. Interpolation. A classical problem in numerical analysis is that of *interpolation*: given the values of a function $f(x)$ at the points $x = x_0$, $x = x_1, \cdots$, $x = x_m$, estimate $f(\bar{x})$, where $\bar{x}$ is a specified point in the interval $[\min_{0 \leqq k \leqq m} x_k, \max_{0 \leqq k \leqq m} x_k]$. If $\bar{x}$ lies outside the interval, the problem is that of *extrapolation.*

The mth order *Lagrangean* method estimates $f(\bar{x})$, for distinct x_k, by

$$f(\bar{x}; x_0, x_1, \cdots, x_m) \equiv f_{0,1,\cdots,m} = \sum_{k=0}^{m} \alpha_k f_k, \tag{36}$$

where

$$\alpha_k = \left(\prod_{\substack{j=0 \\ j \neq k}}^{m} (\bar{x} - x_j) \right) \Big/ \left(\prod_{\substack{j=0 \\ j \neq k}}^{m} (x_k - x_j) \right) \tag{37}$$

and

$$f_k = f(x_k) = f(\bar{x}; x_k).$$

When $m = 1$, we have *linear* interpolation:

$$f(\bar{x}) \doteq f_{0,1} = \frac{(x_1 - \bar{x}) f_0 - (x_0 - \bar{x}) f_1}{x_1 - x_0}. \tag{38}$$

Lagrange's method is very laborious to use, especially if we have to interpolate at several different points, or if we wish to include additional points and hence obtain higher order approximations as checks. We can obtain the same results while avoiding these difficulties by using *Newton's divided difference interpolation formula*:

$$f_{0,1,\ldots,m} = f_0 + \sum_{k=1}^{m} p_k(\bar{x}) \times [x_0, x_1, \cdots, x_k], \tag{39}$$

where

$$p_k(x) \equiv \prod_{j=0}^{k-1} (x - x_j), \qquad k = 1, 2, \cdots, m,$$

$$[x_0, x_1] \equiv \frac{f_1 - f_0}{x_1 - x_0},$$

$$[x_0, x_1, x_2] \equiv \frac{[x_1, x_2] - [x_0, x_1]}{x_2 - x_0}, \tag{40}$$

and

$$[x_0, x_1, \cdots, x_k] \equiv \frac{[x_1, x_2, \cdots, x_k] - [x_0, x_1, \cdots, x_{k-1}]}{x_k - x_0}$$

is the kth order divided difference.

If $x_0 = x_1 = \cdots = x_k$, then

$$[x_0, x_1, \cdots, x_k] = \frac{f^{(k)}(x_0)}{k!}. \tag{41}$$

When the points are equally spaced—i.e., $x_k = x_0 + kh$ for $k = 1, 2, \cdots, m$—and $\bar{x} = x_0 + ph$, we obtain *Newton's forward difference interpolation formula*:

$$f_{0,1,\cdots,m} = f_0 + p\Delta f_0 + \binom{p}{2}\Delta^2 f_0 + \cdots + \binom{p}{k}\Delta^k f_0 + \cdots + \binom{p}{m}\Delta^m f_0, \tag{42}$$

where $\Delta f_0 = f_1 - f_0$, $\Delta^2 f_0 = f_2 - 2f_1 + f_0$, etc.

JORDAN (1928a, b, 1950) attempted to avoid the use of differences and still escape the labor of Lagrange's method by expressing $f_{0,1,\cdots,m}$, for an *even* number of *equally spaced* x_k, as a linear combination of linear interpolates, thus:

$$f_{0,1,\cdots,m} = \sum_{k=0}^{\mu} \binom{p - \mu + k - 1}{2k} V_k, \tag{43}$$

where

$$V_0 = U_0, \qquad V_1 = U_1 - U_0,$$

$$V_2 = U_2 - 3U_1 + 2U_0, \quad \text{etc.},$$

$$U_k = ((\mu + k + 1 - p)f_{\mu-k} - (\mu - k - p)f_{\mu+k+1})/(2k + 1)$$

for $k = 0, 1, \cdots, \mu$ (the linear interpolate between $f_{\mu-k}$ and $f_{\mu+k+1}$), and $m = 2\mu + 1$ (see also LIDSTONE (1932), WISHART (1932)).

However, as AITKEN (1932a) pointed out, the V_i are obtained most readily as differences of increasing order of the series $\cdots U_2, U_1, U_0, U_0, U_1, U_2, \cdots$ (see Table 3), so we have not entirely avoided the use of differences!

TABLE 3

$\vdots$				
U_2				
U_1	$-U_2 + U_1$			
U_0	$-U_1 + U_0$	$U_2 - 2U_1 + U_0$		
$U_0 = V_0$	0	$U_1 - U_0$	$-U_2 + 3U_1 - 2U_0$	
U_1	$U_1 - U_0 = V_1$	$U_1 - U_0 = V_1$	0	$U_2 - 3U_1 + 2U_0$
U_2	$U_2 - U_1$	$U_2 - 2U_1 + U_0$	$U_2 - 3U_1 + 2U_0 = V_2$	$U_2 - 3U_1 + 2U_0 = V_2$
$\vdots$				

Aitken realized that the practical advantage of Jordan's method lay in the simplicity of the process of linear interpolation, and devised a method of "interpolation by iteration" (AITKEN (1932b)) which dispenses completely with the use of differences and which is applicable to *arbitrarily spaced* data. He eliminated $[x_0, x_1, x_2, x_3]$ from

$$f_{0,1,2,3} = f_{0,1,2} + (\bar{x} - x_0)(\bar{x} - x_1)(\bar{x} - x_2) \times [x_0, x_1, x_2, x_3]$$

(easily verified from (39)) and

$$f_{0,1,2,3} = f_{0,1,3} + (\bar{x} - x_0)(\bar{x} - x_1)(\bar{x} - x_3) \times [x_0, x_1, x_2, x_3],$$

obtaining

$$f_{0,1,2,3} = \frac{(x_3 - \bar{x})f_{0,1,2} - (x_2 - \bar{x})f_{0,1,3}}{x_3 - x_2}. \tag{44}$$

Thus $f_{0,1,2,3}$ can be obtained by *linear interpolation* between $f_{0,1,2}$ and $f_{0,1,3}$, etc. (compare (38)).

The successive interpolants can be tabulated in a triangular scheme in which each member of the rth column is the value at $x = \bar{x}$ of an interpolating polynomial of degree r which coincides with $f(x)$ at $r + 1$ points (see Table 4). Each element is formed by linear interpolation between the element in the previous column and same row and the element at the head of the previous column.

TABLE 4

x_0	f_0					
x_1	f_1	$f_{0,1}$				
x_2	f_2	$f_{0,2}$	$f_{0,1,2}$			
x_3	f_3	$f_{0,3}$	$f_{0,1,3}$	$f_{0,1,2,3}$		
...	...	...	...	...		
x_{m-1}	f_{m-1}	$f_{0,m-1}$	$f_{0,1,m-1}$	$f_{0,1,2,m-1}$	...	
x_m	f_m	$f_{0,m}$	$f_{0,1,m}$	$f_{0,1,2,m}$	...	$f_{0,1,\cdots,m}$

Since the interpolating polynomial of degree r through $r + 1$ points is unique (Henrici (1964, p. 183)), each element in the Aitken table is identical with the value obtained by Lagrange's method using the same points. However, the labor has been reduced considerably, and it is much easier to incorporate extra points, computing approximations of higher order until convergence is obtained. Aitken also applied his method to interpolation of functions of two variables and to inverse interpolation (see also KINCAID (1948)).

Aitken observed that, if the data are symmetrically placed, say $x_0 \pm h_0$, $x_0 \pm h_1, \cdots$, then

$$f(\bar{x}; x_0 - h_k, x_0 + h_k) = ((x_0 + h_k - \bar{x})f(\bar{x}; x_0 - h_k) - (x_0 - h_k - \bar{x})f(\bar{x}; x_0 + h_k))/2h_k$$

is an even function of h_k. Consequently we can apply linear interpolation with variable h_k^2 to the functions

$$f(\bar{x}; h_k^2) \equiv f(\bar{x}; x_0 - h_k, x_0 + h_k).$$

Thus

$$f(\bar{x}; h_0^2, h_1^2) = \frac{(h_1^2 - (\bar{x} - x_0)^2) f(\bar{x}; h_0^2) - (h_0^2 - (\bar{x} - x_0)^2) f(\bar{x}; h_1^2)}{h_1^2 - h_0^2} \tag{45}$$

etc. Aitken suggested taking $h_0^2, h_1^2, \cdots$ in increasing order and noted that, if $\bar{x} = x_0 = 0$, "the first quadratic approximation coincides with a process which has been called by L. F. Richardson 'h^2-extrapolation'," i.e.,

$$f(0; h_0^2, h_1^2) = \frac{h_1^2 f(0; h_0^2) - h_0^2 f(0; h_1^2)}{h_1^2 - h_0^2}$$

(compare (30)).

NEVILLE (1932a, 1934) proposed a process of "iterative interpolation" which differed from Aitken's in that every element in the rth column is obtained by linear interpolation between two *adjoining* elements in the $(r-1)$th column, leading to a more symmetrical scheme (see Table 5). In this case we have, for example,

$$f_{0,1,2,3} = \frac{(x_3 - \bar{x}) f_{0,1,2} - (x_0 - \bar{x}) f_{1,2,3}}{x_3 - x_0} \tag{46}$$

(compare (44)). The elements in the leading diagonal are identical in the two schemes, but the convergence behavior elsewhere, which depends on the ordering of the x_k, will differ.

TABLE 5

x_0	f_0					
x_1	f_1	$f_{0,1}$				
x_2	f_2	$f_{1,2}$	$f_{0,1,2}$			
x_3	f_3	$f_{2,3}$	$f_{1,2,3}$	$f_{0,1,2,3}$		
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$		
x_{m-1}	f_{m-1}	$f_{m-2,m-1}$	$f_{m-3,m-2,m-1}$	$f_{m-4,m-3,m-2,m-1}$	$\cdots$	
x_m	f_m	$f_{m-1,m}$	$f_{m-2,m-1,m}$	$f_{m-3,m-2,m-1,m}$	$\cdots$	$f_{0,1,\cdots,m}$

A great advantage of Neville's process is that it is easy to incorporate derivative values by the limiting cases:

$$\begin{aligned} f_{k,k} &= f_k + (\bar{x} - x_k) f'(x_k), \\ f_{k,k,k} &= f_{k,k} + \tfrac{1}{2}(\bar{x} - x_k)^2 f''(x_k), \end{aligned} \tag{47}$$

etc. Thus if we know $f(x_0), f(x_1), f'(x_1), f''(x_1), f(x_2), f(x_3)$, and $f'(x_3)$, we can use the scheme in Table 6 to interpolate for $f(\bar{x})$, where the underlined elements are obtained by using (47).

TABLE 6

x_0	f_0						
x_1	f_1	$f_{0,1}$					
x_1	f_1	$\underline{f_{1,1}}$	$f_{0,1,1}$				
x_1	f_1	$\underline{f_{1,1}}$	$\underline{f_{1,1,1}}$	$f_{0,1,1,1}$			
x_2	f_2	$f_{1,2}$	$f_{1,1,2}$	$f_{1,1,1,2}$	$f_{0,1,1,1,2}$		
x_3	f_3	$f_{2,3}$	$f_{1,2,3}$	$f_{1,1,2,3}$	$f_{1,1,1,2,3}$	$f_{0,1,1,1,2,3}$	
x_3	f_3	$\underline{f_{3,3}}$	$f_{2,3,3}$	$f_{1,2,3,3}$	$f_{1,1,2,3,3}$	$f_{1,1,1,2,3,3}$	$f_{0,1,1,1,2,3,3}$

6. Further developments. Between 1933 and 1955 there were many modifications, extensions and applications of the methods of §§ 2 to 5. Some of these developments are reviewed in this section.

MILNE–THOMSON (1933, p. 99) noticed that Boole's rule can be obtained by eliminating the term in h^4 between two Simpson values:

$$B(h) = (16S(h) - S(2h))/15. \tag{48}$$

(RUNGE and KÖNIG (1924) had noted that

$$I - S(h) \doteq (S(h) - S(2h))/15$$

but had not suggested using this as a *correction.*) KOMMERELL (1935) proved that all Milne's approximations to π (see § 2) satisfy

$$T(h, h/2, \cdots, h/2^m) < \pi$$

and that

$$T(h, h/2, h/4) = (16S(h/4) - S(h/2))/15$$

(compare (48)).

HARTREE and WOMERSLEY (1937) suggested solving partial differential equations (PDE's) of parabolic type with the help of finite difference methods and improving the approximate solutions by h^2-extrapolation. They pointed out that the latter was only valid for certain types of boundary conditions and could then be applied *locally*, i.e., after advancing from x to $x + 2h$ using h and $2h$, or *globally*, after covering the whole range using h and $2h$.

LIDSTONE (1937) discussed Aitken's method in detail (as did FELLER (1943)), introducing the terms "linear cross mean" (for (44)) and "quadratic cross mean" (for (45)). AITKEN (1938) showed how quadratic cross means (QCM's) can be used in numerical differentiation with symmetrically placed data. Differentiating $f(x; h_0^2, h_1^2)$ s times with respect to x and setting $x = \bar{x}$, we obtain

$$\begin{aligned} f^{(s)}(\bar{x}; h_0^2, h_1^2) = ((h_1^2 - X^2)f_0^{(s)} - (h_0^2 - X^2)f_1^{(s)} - 2sX(f_0^{(s-1)} - f_1^{(s-1)}) \\ - s(s-1)(f_0^{(s-2)} - f_1^{(s-2)}))/(h_1^2 - h_0^2), \end{aligned} \tag{49}$$

where $X = \bar{x} - x_0$ and $f_r^{(q)} = f^{(q)}(\bar{x}; h_r^2)$ for $q = s, s-1, s-2$ and $r = 0, 1$. To approximate $f^{(s)}(\bar{x})$, $s + 1$ tables are required (for $f, f', f'', \cdots, f^{(s)}$). The table for f' has

$$f'(\bar{x}; h_k^2) = (f(x_0 + h_k) - f(x_0 - h_k))/(2h_k) \tag{50}$$

and the table for $f^{(q)}$ has zeros in the first $[q/2]$ columns. The other elements are constructed from relations like (49). Aitken also showed how QCM's can be used in inverse interpolation.

BICKLEY (1939) observed that the Newton–Cotes 7-point rule can be obtained by combining $W(h)$ (from (15)) and $H(h)$ (from (16)). ZURMUHL (1940) used $(T(h) - T(2h))/15$ as a *correction* in applying the method of Nystrom (1925) to $y'' = f(x, y, y')$. BUCKNER (1948) showed that, when a symmetric difference method

is used to obtain an approximate solution, $\Lambda = \Lambda(h)$, of the differential eigenvalue (EV) problem

$$(r(x)y'(x))' + (\lambda p(x) + q(x))y = 0,$$

with $y(a) = y(b) = 0$, the error in Λ satisfies

$$\Lambda(h) - \lambda = a_1 h^2 + O(h^4). \tag{51}$$

He noted that h^2-extrapolation is valid in this case and that a more accurate difference method will allow h^4-extrapolation.

DUNCAN (1947, 1948a, b) proposed solving initial value (IV) problems in ODE's according to the following strategy:

(a) estimate the step, h_1, required to obtain the prescribed accuracy using the chosen pth order discretization process;

(b) compute $T(h_1)$ and $T(h_0)$, with $h_0 > h_1 (h_0 = 2h_1$, say);

(c) if the correction

$$T(h_0, h_1) - T(h_1) = \frac{(T(h_0) - T(h_1))h_1^p}{h_1^p - h_0^p}$$

is too large, compute $T(h_2)$, with $h_2 < h_1$ ($h_2 = h_1/2$, say), and hence $T(h_0, h_2)$, $T(h_1, h_2)$ and $T(h_0, h_1, h_2)$.

Duncan used this strategy with *Euler's method* (Euler (1768)),

$$Y_{r+1} = Y_r + hf(x_r, Y_r), \tag{52}$$

for which $p = 1$, and with the *modified Euler method*,

$$Y_{r+1} = Y_r + hf(x_{r+1/2}, Y_r + \tfrac{1}{2}hf(x_r, Y_r)), \tag{53}$$

for which $p = 2$. He also observed that a similar strategy can sometimes be applied to problems involving PDE's.

RUBBERT (1949) investigated the use in quadrature of "enclosing formulas"—i.e., pairs of formulas of the same order of accuracy whose errors have leading terms of opposite sign. For example, he paired $S(h)$ with a method of Maclaurin type (Kowalewski (1932)):

$$K(h) = \tfrac{1}{4}h\{3f_{1/3} + 2f_1 + 3f_{5/3} + 3f_{7/3} + 2f_3 + \cdots + 2f_{n-1} + 3f_{n-1/3}\}. \tag{54}$$

Now

$$S(h) - I = 18(b - a)h^4 f^{\mathrm{iv}}(\xi_1)/3240,$$

and

$$K(h) - I = -7(b - a)h^4 f^{\mathrm{iv}}(\xi_2)/3240,$$

where $a < \xi_i < b$, so, if

$$f^{\mathrm{iv}}(\xi_1) \times f^{\mathrm{iv}}(\xi_2) > 0,$$

we have

$$(S(h) - I) \times (K(h) - I) < 0;$$

i.e., $S(h)$ and $K(h)$ enclose the exact value I.

He proposed using $(3K(h) + S(h))/4$, which has a very small coefficient of h^4 in its error, as an improved value (compare (27)). Similarly he paired the 3- and 4-point Gauss formulas (Stroud and Secrest (1966, p. 100)), G_3 and G_4, with the 4- and 5-point Lobatto formulas (Ibid., p. 318), L_4 and L_5, using $(4G_3 + 3L_4)/7$ and $(5G_4 + 4L_5)/9$ as improved values. In each case the leading term in the error has been eliminated, since $(n + 1)(G_n - I) \doteq -n(L_{n+1} - I)$ (see Filippi (1964)). MILNE (1949) used a similar idea with predictor-corrector methods for IV problems in ODE's.

SALVADORI (1949a, b) used central difference formulas to compute buckling loads—i.e., solve linear differential EV problems. He observed that the approach of the approximate solution, $\Lambda(h)$, to the exact solution, λ, as $h \to 0$, was often monotonic, sometimes oscillatory and sometimes one-sided but not monotonic, but that in every case a decreasing sequence $\{h_k\}$ could be chosen such that $\{\Lambda(h_k)\}$ was monotonic.

His experiments supported the hypothesis that, when central difference approximations are used, the error in Λ is usually "of the h^{2p}-type," i.e.,

$$\Lambda(h) - \lambda = a_1 h^{2p} + a_2 h^{2p+2} + a_3 h^{2p+4} + \cdots \tag{55}$$

($p = 1, 2, \cdots$, depending on the order of approximation employed). Thus the deferred approach to the limit can be used to obtain, for example,

$$\Lambda(h_0, h_1, \cdots, h_m) = \sum_{k=0}^{m} \alpha_k \Lambda(h_k). \tag{56}$$

When $p = 1$, the α_k are defined by (20).

Salvadori tabulated the coefficients α_k for h^2-, (h^2, h^4)-, h^4- and (h^4, h^6)-extrapolation (for a variety of $\{r_k\}$) and applied them successfully to buckling problems in one and two dimensions. For boundary conditions involving a derivative he used the same order approximation as for the DE (NEWMARK (1949) observed that, if a higher order approximation is used for the DE, odd powers of h may appear).

FOX (1950) compared the "deferred approach to the limit" with the method of "difference corrections" as ways of improving the approximate solutions of elliptic PDE's. HERRMANN (1951) used skew and triangular coordinates in computing the deflections of a skew plate and obtained approximations from above and below for extrapolation.

WANG (1951) and SALVADORI (1951a) attempted to prove that "the error in the characteristic value of linear ODE's with constant coefficients evaluated by finite differences is of the h^2-type." Salvadori noted that the experimental evidence indicated that this was not usually true for equations with *variable* coefficients. He noted that "the extrapolations can actually be used in connection with any method of successive approximations in which the successive values of the un-

known depend on an increasing integer n and the error is expandable into a series of even negative powers of n."

In a conference paper (SALVADORI (1951b)) and a textbook (SALVADORI and BARON (1952)) he applied the extrapolations to:

(a) numerical differentiation: h^2- and (h^2, h^4)-extrapolation of

$$f'(\bar{x}; h) = (f(\bar{x} + h) - f(\bar{x} - h))/(2h) \tag{57}$$

(compare (50));

(b) numerical integration: h^2- and (h^2, h^4)-extrapolation of $T(h)$ and the product trapezium rule, h^4-extrapolation of $S(h)$ and the product Simpson rule;

(c) boundary value (BV) and eigenvalue (EV) problems in ODE's and PDE's (see also RAMASWAMY (1951)).

He noted the following points:

(a) It is not known in general whether the extrapolants are approximations from above or below (see also BOLEY (1951)).

(b) It is unsafe to use the extrapolations without at least 3 approximate values.

(c) The extrapolations should not be used when the successive approximations do not approach the true value monotonically, since in this case the higher terms of the error series cannot be neglected.

(d) If the approach is oscillatory, the methods may be applied separately to the approximations from above and below, and the results compared.

CULVER (1952) used electrical resistance networks to solve the central difference approximations of Laplace's equation and applied h^2- and (h^2, h^4)-extrapolation to the results in order to obtain high accuracy without using a larger network (see also LIEBMANN (1950), who used h^2-extrapolation only). He noted that the quality of the final results depends critically on the accuracy of the original approximations and suggested a ratio test to determine whether the higher terms are negligible. BLANCH (1953) investigated the use of extrapolation in the numerical solution of parabolic PDE's (see also BATTEN (1961), DOUGLAS (1961)). FOX and GOODWIN (1953) applied h^2- and (h^2, h^4)-extrapolation to improve the approximate solutions, obtained by use of the trapezium rule, of integral equations (IE's) of various types.

TWEEDIE (1954) suggested a modification of the Aitken–Neville process to be used when the numbers of points on either side of $\bar{x}$ are equal or differ by one. His scheme makes fullest use of the points nearest $\bar{x}$ from the earliest stages and uses them for interpolation rather than extrapolation (see Table 7, where $x_0 < x_1 < x_2 < \bar{x} < x_3 < x_4 < x_5$). Usually there is less variation in the early columns than in Aitken's or Neville's schemes.

TABLE 7

x_0	f_0					
x_1	f_1	$f_{0,3}$				
x_2	f_2	$f_{1,3}$	$f_{0,2,3}$			
x_3	f_3	$f_{2,3}$	$f_{1,2,3}$	$f_{0,2,3,4}$		
x_4	f_4	$f_{2,4}$	$f_{2,3,4}$	$f_{1,2,3,4}$	$f_{0,1,2,3,4}$	
x_5	f_5	$f_{2,5}$	$f_{2,3,5}$	$f_{1,2,3,5}$	$f_{1,2,3,4,5}$	$f_{0,1,2,3,4,5}$

GORN (1954) noted that h^p-extrapolation of the results of applying a pth order discretization process to an IV problem in ODE's can be used (globally or locally) to provide an error estimate and/or an improved value (see also GORN and MOORE (1953), GARFINKEL (1954), LOTKIN (1955), ROMANELLI (1960), PROTHERO (1969)). A local error estimate can be used for step size control (see, e.g., FEHLBERG (1969)). He described an algorithm which made use of extrapolation to provide two enclosing solutions.

SALZER (1954, 1956) used extrapolation to evaluate the Nth term or the limit of a sequence. He assumed (like Richardson (32)) that

$$T_n = a_0 + a_1/n + a_2/n^2 + \cdots,$$

where T_n is the nth element of the sequence, and approximated T_N by $\sum_{k=i}^{i+m} \alpha_k T_k$, where the α_k are the Lagrangean coefficients (see (37)) for $x_k = 1/k$ and $\bar{x} = 1/N$ ($\bar{x} = 0$ for limits). He tabulated the α_k for a variety of i and m (WYNN (1956b) used divided differences instead). By defining T_n to be the nth partial sum of a series, the method can be used to sum (partially or completely) series. If the terms in the series vary in sign or oscillate in size, the method is still applicable provided the terms are grouped suitably.

WASOW (1955) pointed out that "except for domains with very special boundaries, the benefit to be expected from the use of Richardson's idea in the numerical solution of Dirichlet's problem" (a general BV problem in PDE's) "depends decisively on the interpolation formula employed near the boundary." This is not a problem for rectangular boundaries (thus Richardson and Salvadori did not encounter it), but, when the boundary is curved, extrapolation may be valueless unless use is made of a more refined interpolation formula than would otherwise be necessary (see also HUBBARD (1966)).

KOPAL (1955) noted that, in discretization processes, as $h \to 0$ the discretization error decreases, but the rounding error increases. He saw the deferred approach to the limit as a way of reducing the discretization error without significantly increasing either the rounding error or the amount of work, and applied it to the EV problem in ODE's.

7. Iterative linear extrapolation. ROMBERG (1955) appears to have been the first to see that the error term elimination processes of § 3 (above) can be effected by iterative linear extrapolation. Let us define, for $i, m = 0, 1, 2, \cdots$,

$$T_m^i = T(h_i, h_{i+1}, \cdots, h_{i+m}) \tag{58}$$

and

$$U_m^i = U(h_i, h_{i+1}, \cdots, h_{i+m}), \tag{59}$$

so that T_0^i is the trapezoidal value $T(h_i)$ and U_0^i is the midpoint value $U(h_i)$ (this notation is more flexible than Romberg's). Romberg showed that, when $h_{i+s} = 2^{-s}h_i$ for $s = 1, 2, \cdots, m$ and $i = 0, 1, 2, \cdots$, we have for $i = 0, 1, 2, \cdots$, and $m = 1, 2, 3, \cdots$,

$$T_m^i = T_{m-1}^{i+1} + (T_{m-1}^{i+1} - T_{m-1}^i)/(4^m - 1) \tag{60}$$

(for $m = 1, 2$ this is equivalent to (21), (48)), and

$$U_m^i = U_{m-1}^{i+1} + (U_{m-1}^{i+1} - U_{m-1}^i)/(4^m - 1), \tag{61}$$

and that for $i = 1, 2, 3, \cdots$ and $m = 0, 1, 2, \cdots$,

$$T_m^i = (T_m^{i-1} + U_m^{i-1})/2 \tag{62}$$

(for $m = 0$ this is equivalent to (24)).

The T_m^i and U_m^i can be arranged in a triangular scheme (Table 8) similar to Neville's.

TABLE 8

h_0	T_0^0 [11]			
	U_0^0 [23]			
h_1	T_0^1 [62]	T_1^0 [60]		
	U_0^1 [23]	U_1^0 [61]		
h_2	T_0^2 [62]	T_1^1 [62]	T_2^0 [60]	
	U_0^2 [23]	U_1^1 [61]	U_2^0 [61]	
h_3	T_0^3 [62]	T_1^2 [62]	T_2^1 [62]	T_3^0 [60]

The table is built up row by row, from left to right, using the equations indicated in brackets after each entry. Note that, for $m > 0$ and $i > 0$, the T_m^i are obtained from (62) and not from (60), thus reducing the labor. Although this method is equivalent to the methods of § 3 (above) the coefficients α_k in (19) are not computed explicitly after the first extrapolation; thus Romberg's method has the same advantages over the methods of § 3 (above) that Neville's process has over Lagrange's method of interpolation.

Romberg observed that the leading term in the error expansion of T_m^i has the same order as that of U_m^i but the opposite sign. Thus, if the leading term is dominant in each expansion, the true value, I, will be between T_m^i and U_m^i, and T_m^{i+1} will usually be more accurate than either.

A disadvantage of using a sequence $\{h_k = r_k h\}$ in geometric progression is that the number of function values used increases exponentially with increasing order. Romberg noted that 12, although smaller than 16, has one more divisor, thus allowing the elimination of an additional power of h^2. Let us denote the divisors of an integer n by $\{d_0(n), d_1(n), \cdots, d_\nu(n)\}$, with $1 = d_0(n) < d_1(n) < \cdots < d_\nu(n) = n$; then we have

$$\{d_k(12)\} = \{1, 2, 3, 4, 6, 12\}, \qquad \{d_k(16)\} = \{1, 2, 4, 8, 16\}.$$

Now the function values required for $T(h)$, $T(h/2)$, $T(h/3)$, $T(h/4)$, $T(h/6)$ are all used in $T(h/12)$; thus, by using $r_k = 1/d_k(12)$ instead of $r_k = 1/d_k(16)$, we can obtain an approximation of order two higher for $\frac{3}{4}$ of the number of function evaluations. Of course, the formulas equivalent to (60), (61) and (62) are more complicated; nevertheless (as COREY (1906) pointed out (see § 3)), there are advantages in choosing $r_k = 1/d_k(n)$ for some number n which has a relatively high number of divisors.

If function evaluation is difficult, Romberg suggested using extrapolations on higher order methods, for example the pair

$$T^*(h) \equiv T(h) + A(h) = T(h) + \tfrac{1}{24}h(f_1 - f_{-1} + f_{n-1} - f_{n+1}) \tag{63}$$

and

$$U^*(h) \equiv U(h) - 2A(h/2) \tag{64}$$

(Amble (1952)), which have errors of h^4-type (compare (26)).

BOLTON and SCOINS (1956, 1957) made use of Neville's process twice in solving the EV problem for Schrödinger's equation in one and two dimensions. Firstly, having used a central difference approximation to obtain the algebraic EV problem

$$\Delta(\Lambda) \equiv |A - \Lambda I| = 0, \tag{65}$$

they solved for $\Lambda = \Lambda(h)$ by iterative inverse interpolation, improving estimates Λ_0 and Λ_1 according to

$$\Lambda_{0,1} = \frac{\Delta_1\Lambda_0 - \Delta_0\Lambda_1}{\Delta_1 - \Delta_0} \tag{66}$$

and then obtaining $\Lambda_{0,1,2}$ etc. Secondly, they improved the approximate eigenvalues $\Lambda(h_k)$, where $h_k = 1/n_k$, n_k an integer, using, for example,

$$\Lambda(h_0, h_1, h_2) = \frac{h_2^2\Lambda(h_0, h_1) - h_0^2\Lambda(h_1, h_2)}{h_2^2 - h_0^2}. \tag{67}$$

This second application of Neville's process is equivalent to the methods of Richardson (who solved linear equations (see § 4 (above)) and Salvadori (who obtained explicit coefficients (see § 6 (above)), but rather more elegant.

Bolton and Scoins showed that, under certain conditions;

$$\Lambda(h) = \lambda + a_1h^2 + O(h^4)$$

(compare (51)), with a_1 usually negative, and hypothesized from symmetry that the error in $\Lambda(h)$ is of the h^2-type, which justifies the use of extrapolation. They pointed out that "since the numerical rounding errors quickly build up, it is dangerous to extend the Neville table too far, particularly when the values of n_k are close together" (they used $\{2, 3, 4, \cdots\}$), and that the coarsest approximation, $\Lambda(\frac{1}{2})$, may be misleading for extrapolation.

EVE and SCOINS (1956) investigated the approximate solution, by symmetric difference methods, of the PDE's of Laplace and Poisson. They found that under certain conditions, if we use $T(h)$ and $U(h)$ to denote the approximations obtained using "square" and "diagonal" grids, the error expansions are

$$T(h) - a_0 = a_1h^2 + a_2h^4 + a_3h^6 + \cdots$$

and

$$U(h) - a_0 = -a_1h^2 + a_2h^4 - a_3h^6 + \cdots.$$

Thus extrapolation in h^2 can be carried out using a modified form of Neville's process, with T and U values alternating in the first column.

8. Other developments. Little notice seems to have been taken of the advances made by Romberg, Bolton and Scoins until 1961. In the intervening 5 years there were some developments, mostly related to the use of extrapolation methods in the solution of DE's.

CRANDALL (1956) discussed the use of extrapolation to improve approximate solutions of IV and BV problems in ODE's and PDE's. LISTER and ROBERTS (1956) showed that extrapolation could be employed in the numerical solution of hyperbolic PDE's (see also ROBERTS (1958), LISTER (1960)). HILDEBRAND (1956) observed that h^4-extrapolation does not improve Simpson's rule approximations to $\int_{-4}^{4}(1+x^2)^{-1}\,dx$. In this case, the $S(h)$ values oscillate as h decreases.

DE VOGELAERE (1957) generalized Gaunt's special starting procedure (see § 4 (above)) so that $(h^2, h^4, \cdots, h^{2m})$-extrapolation could be used to improve approximate solutions of

$$y' = f(x, y), \qquad y(x_0) = y_0, \tag{68}$$

and

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y_0', \tag{69}$$

obtained by the midpoint method (35). The extrapolation will not usually be valid if Runge–Kutta or Taylor series methods are used to take the first step, nor if the exact value is used. However, his starting procedures require the values of $2m$ derivatives, which may not be easily obtainable.

FOX (1957, 1961, 1962) showed how the form of the error in the approximate solution of a DE problem can be determined. Concerning ODE problems, he observed that "if the rounding error is ignored, if the solution is sufficiently well-behaved, and if the interval is small enough... it seems likely that the error at any point is expressible as a power series in h." His method, which is based on introducing such expansions into the corresponding discrete problem and equating coefficients of powers of h, is also applicable to PDE problems.

The error will usually be of the h^{2p}-type if central difference methods are used to approximate the DE and the boundary conditions. However, Fox pointed out that, although

$$xy'' - y' - x = 0 \tag{70}$$

and

$$x^2y'' - 2y - 1.5x^2 = 0 \tag{71}$$

have the same solution if $y(0) = y(1) = 0$, when central difference methods are used h^2-extrapolation seems valid for (71) but not for (70) (MAYERS (1964) showed that the error for (70) has terms in $h^2 \ln h$ etc.). Thus "the validity of extrapolation would seem to depend on the form of the DE as well as its solution" (see also FOX and MAYERS (1968)).

Fox also noted that "consistent inaccuracy" may occur; i.e., successive extrapolants may agree within ε while having errors very much greater than ε, and that the usual extrapolations may not be valid if the boundary is curved or there are discontinuities, singularities or awkward corners. FORSYTHE and WASOW (1960, p. 351) quote a conjecture of de Vogelaere's that for the L-shaped membrane eigenvalue problem, as $h \to 0$,

$$\Lambda(h) - \lambda = a_1h^{4/3} + a_2h^2 \ln h + a_3h^2 + a_4h^{8/3} + \cdots. \tag{72}$$

OSBORNE (1960) used Fox's technique to demonstrate that, when central difference approximations are used in the EV problem for second order self-adjoint ODE's, the errors in Λ and T are of h^2-type. He then solved for a_1, etc. before correcting. FOX (1960) and SYLVESTER and FOLL (1960) also used extrapolation in solving EV problems in ODE's.

HENRICI (1960, 1962, 1963a, b) showed that, when a pth order "one-step" discretization method is used to solve the ODE's (34), under certain conditions of continuity and differentiability, the error in the approximate solution has the asymptotic behavior, as $h \to 0$,

$$T(h) - a_0 = a_1 h^p + O(h^{p+1}) \tag{73}$$

with a_1 independent of h and satisfying a DE. This result holds true for variable step size (see also LETHER (1966)). Henrici asserted that "from a mathematical point of view this may be regarded as the first term of an asymptotic expansion" of form (1) with $\gamma_j = p + j - 1$. When a "multistep" method is used, $a_1(x)$ will be dependent on h unless the method is "strongly stable" (i.e., there is only one "essential root").

HUNTER (1961) proposed an iterative method of numerical differentiation which, unlike Aitken's (see § 6), can be used with arbitrarily spaced data. The equation corresponding to (49) is

$$\begin{aligned} f^{(s)}(\bar{x}; x_0, x_1) = ((x_1 - \bar{x})f^{(s)}(\bar{x}; x_0) - (x_0 - \bar{x})f^{(s)}(\bar{x}; x_1) \\ - s(f^{(s-1)}(\bar{x}; x_0) - f^{(s-1)}(\bar{x}; x_1)))/(x_1 - x_0), \end{aligned} \tag{74}$$

and the tables are constructed in a similar way to Aitken's (see also GERSHINSKY and LEVINE (1964), LAURENT (1964b), LYNESS and MOLER (1966), KROGH (1970)). THACHER (1962b) used an analogous method for repeated quadrature.

SALZER and KIMBRO (1961) showed that extrapolation in $1/n^2$ can be used for complete or partial summation of series provided the nth partial sum T_n behaves like an even function of n. Subsequently SALZER (1961) published an interpolation formula for "nearly-odd" functions and applied it to the summation of even functions.

9. Analysis of Romberg's method. BAUER (1961a) seems to have been the first to produce a rigorous error analysis of Romberg's method. Using certain periodic functions, he was able to prove that, if $f(x)$ has $2m + 2$ continuous derivatives on $[0, 1]$ (i.e., $f(x) \in C_{2m+2}[0, 1]$), and $h_k = 2^{-k}$, then

$$T_m^0 - \int_0^1 f(x)\,dx = \frac{\beta_{m+1} f^{(2m+2)}(\xi)}{2^{m(m+1)}}, \tag{75}$$

with $0 \leqq \xi \leqq 1$. This implies that $\{T_m^0\}$ converges *superlinearly* as $m \to \infty$ (in fact, $T_m^0 - \int_0^1 f(x)\,dx \sim 2f^{(2m+2)}(\xi)/(2^{m+2}\pi^2)^{m+1}$). He also obtained conditions under which T_m^0 and U_m^0 will enclose the true value $\int_0^1 f(x)\,dx$, noting that this will be true if $f^{(2m+2)}(x)$ does not change sign in $[0, 1]$, and pointed out that T_m^i can be computed from

$$T_m^i = U_m^i + (\tfrac{1}{2}4^m - 1)(T_{m-1}^i - U_{m-1}^i)/(4^m - 1). \tag{76}$$

Bauer observed that Romberg's method has the following advantages over Newton–Cotes methods:

(a) explicit weights are not required but are positive (some higher order Newton–Cotes methods have negative weights);

(b) the order is increased very easily;

(c) the method is admirably suited for automatic computation.

Finally, he noted that it can easily be extended to integration in several dimensions.

RUTISHAUSER and STIEFEL (1961) and STIEFEL (1961) presented the following results for $I = \int_a^b f(x)\,dx$, $h = b - a$ and $r_k = 2^{-k}$:

(a) There exist continuous functions for which the Newton–Cotes values do not converge with increasing order (Kusmin (1931), Polya (1933), Davis (1955, 1962)).

(b) If $f(x)$ is sufficiently differentiable and $f'(a) \neq f'(b)$, then $\{T_0^i\}$ converges linearly to I with increasing i (convergence factor $\frac{1}{4}$).

(c) If we write T_m^i as a weighted sum of function values

$$T_m^i = \sum_{r=0}^{n}{}'' w_r f_r = \{\tfrac{1}{2}w_0 f_0 + w_1 f_1 + \cdots + w_{n-1} f_{n-1} + \tfrac{1}{2}w_n f_n\}, \tag{77}$$

where $n = 2^{i+m}$, then $w_r > 0$ for $r = 0, 1, \cdots, n$.

(d) If $f(x)$ is periodic on $[a, b]$ and regular-analytic in a strip including the x-axis, then $\{T_0^i\}$ converges superlinearly (Davis (1959)).

(e) If $f(x) \in C_0[a, b]$, then $\{T_m^0\}$ converges to I.

(f) If $f(x)$ is regular-analytic in a domain including $[a, b]$, then $\{T_m^0\}$ converges superlinearly.

(g) T_m^0 integrates a polynomial of degree $2m + 1$ exactly (using $2^m + 1$ points to attain the same order as the $(2m + 1)$-point Newton–Cotes formula or $(m + 1)$-point Gaussian formula).

They obtained for $f(x) \in C_{2m+2}[a, b]$,

$$T_m^0 - I = 2(b - a)^{2m+3}\zeta(2m + 2) f^{(2m+2)}(\xi)/(2^{m+2}\pi^2)^{m+1}, \tag{78}$$

where $a \leqq \xi \leqq b$ and $\zeta(2m + 2)$ is the Riemann zeta function (Whittaker and Watson (1927, p. 265)). When $a = 0$ and $b = 1$, this reduces to (75), since $\zeta(2m + 2) = 2^{2m+1}\pi^{2m+2}\beta_{m+1}$.

In a joint paper, BAUER, RUTISHAUSER and STIEFEL (1963) showed that, if we write

$$T_m^i = \sum_{s=i}^{i+m} c_{i,m,s} T_0^s, \tag{79}$$

then, for $r_k = 2^{-k}$,

$$\sum_{s=i}^{i+m} c_{i,m,s} = 1, \tag{80}$$

$$(-)^{i+m-s} c_{i,m,s} > 0, \qquad s = i, i + 1, \cdots, i + m, \tag{81}$$

$$\sum_{s=i}^{i+m} |c_{i,m,s}| < 1.97, \tag{82}$$

and

$$\lim_{m\to\infty} c_{i,m,s} = 0. \tag{83}$$

Inequality (82) guarantees the numerical stability of the method, since, if the maximum rounding error in the trapezoidal values is ε, the rounding error in the extrapolated values, neglecting the rounding error in the extrapolation process, cannot exceed 2ε. Relations (80), (82) and (83) allow a theorem of Toeplitz (1911) to be applied, proving that, if $\{T_0^i\}$ converges, then all columns and diagonals of the Romberg scheme will converge to the same limit (see also FOCK (1967)). This limit will be I if $f(x)$ is Riemann integrable.

They observed that, if we define

$$F(r_k^2) \equiv T(r_k h) = T_0^k,$$

the process can be viewed as Neville's process extrapolation of $\{F(r_k^2)\}$ to $F(0)$. The convergence results proved for $r_k = 2^{-k}$ will hold for general $\{r_k\}$ provided there exists a constant ρ, less than 1, such that $r_{k+1}/r_k < \rho$ for all k (see also LAURENT (1963a, b), who investigated the general deferred approach to the limit, and BULIRSCH (1964)). For instance, the choice

$$\{1, \tfrac{1}{2}, \tfrac{1}{3}, \tfrac{1}{6}, \tfrac{1}{9}, \tfrac{1}{18}, \cdots\} = \{r_k; r_{2k} = 3^{-k}, r_{2k+1} = \tfrac{1}{2}3^{-k}, k \geqq 0\} \tag{84}$$

requires modified recurrence relations (to replace (60), (61) and (62)) and is more susceptible to rounding error (since $\sum_{s=i}^{i+m} |c_{i,m,s}|$ can be as large as 3.5), but may reduce computing time.

They proved that, for $h_k = 2^{-k}$, if $f(x) \in C_{2m+2}[0, 1]$, then

$$T_m^i - \int_0^1 f(x)\,dx = \frac{\beta_{m+1} f^{(2m+2)}(\xi)}{2^{(m+2i)(m+1)}}, \tag{85}$$

with $0 \leqq \xi \leqq 1$ (compare (75)). However, in certain cases (e.g., $\int_{-\infty}^{\infty} e^{-x^2}\,dx$ and $\int_{-\infty}^{\infty} (1 + x^2)^{-1}\,dx$) the error in the trapezoidal rule is not of the h^2-type and Romberg's method may not improve the convergence.

BULIRSCH (1964) generalized (60) to

$$T_m^i = \frac{h_i^2 T_{m-1}^{i+1} - h_{i+m}^2 T_{m-1}^i}{h_i^2 - h_{i+m}^2} \tag{86}$$

and investigated the use of $r_k = 1/(1 + k)$ and the sequence

$$Q = \{1, \tfrac{1}{2}, \tfrac{1}{3}, \tfrac{1}{4}, \tfrac{1}{6}, \tfrac{1}{8}, \cdots\} = \{r_k; r_0 = 1, r_{2k-1} = 2^{-k}, r_{2k} = \tfrac{2}{3}2^{-k}, k \geqq 1\},$$

as well as $r_k = 2^{-k}$. He found that, under certain conditions

$$T_m^0 - \int_0^1 f(x)\,dx = h_0^2 h_1^2 \cdots h_m^2 \beta_{m+1} f^{(2m+2)}(\xi) \tag{87}$$

(see also KANDZIA (1963), BULIRSCH and RUTISHAUSER (1968)) and obtained the analogous result in two dimensions:

$$T_m^0 - \int_0^1 \int_0^1 f(x, y)\,dx\,dy = h_0^2 h_1^2 \cdots h_m^2 S, \tag{88}$$

where $S = \sum_{s=0}^{m+1} \beta_s \beta_{m+1-s} f^{(2m+2-2s,2s)}(\xi_s, \eta_s)$. He used (87) to compare error estimates and function evaluations for all three sequences and concluded that overall, taking into account calculation expense, accuracy and stability, Q is best. He noted that, although the sequence $\{r_k = 1/(1+k)\}$ does not satisfy the "ρ-condition" ($r_{k+1}/r_k \leqq \rho < 1$ for all k) and $\sum_{s=i}^{i+m} |c_{i,m,s}|$ increases without bound as m increases, it may still be useful in practice if we do not need the last figures. FILIPPI (1964, 1965a) also examined the error and convergence behavior of Romberg's method.

10. Integrals with singularities. Much work has been done since 1961 to extend the applicability of extrapolation methods and improve the algorithms used for implementing them. Some of these developments are reviewed in this section and the following sections.

FOX (1961, 1962) observed that the Euler–Maclaurin summation formula (18) and the corresponding formula for $S(h)$ (see (6)) must be modified if any of the derivatives of the integrand become infinite in $[a, b]$. In particular, if this occurs at $x = a$, (18) and (6) can be used for $\int_{a+h}^{b} f(x)\,dx$ and $\int_{a+2h}^{b} f(x)\,dx$, respectively, and the rest of the integral can be obtained by using a Taylor series expansion about $x = a + h$. When $a = 0, b = 1$ (which will be assumed in this section, unless other values are specified) and $f(x) = x \ln x$, the asymptotic error expansion for $T(h)$ has a term in $h^2 \ln h$ as well as $h^2, h^4, \cdots$ and that for $S(h)$ has a term in h^2, as well as $h^4, h^6 \cdots$. If $f(x) = x^{1/2}$, there is a term in $h^{3/2}$ in both expansions.

NAVOT (1961, 1962, 1963) used a similar technique to Fox's to extend the Euler–Maclaurin summation formula for $\int_0^1 f(x)\,dx$ to the *generalized trapezoidal rule*:

$$
\begin{aligned}
R^{[n,\alpha]}f(x) &\equiv \frac{1}{n}\sum_{j=1}^{n} f\left(\frac{2j-1+\alpha}{2h}\right), \qquad |\alpha| < 1, \\
R^{[n,1]}f(x) &\equiv T(h),
\end{aligned}
\tag{89}
$$

where $nh = 1$, applied to integrals with singularities. In particular, for

$$U(h) \equiv R^{[n,0]}f(x)$$

and $T(h)$ (with $f_0 = 0$), he showed that, when $f(x) = x^\beta g(x)$, with $0 > \beta > -1$, the expansions have terms in $h^{1+\beta}, h^{2+\beta}, \cdots$, as well as $h^2, h^4, \cdots$ and when $f(x) = x^\beta \ln x\, g(x)$, there are terms in $h^{1+\beta} \ln h, h^{1+\beta}, h^{2+\beta} \ln h, h^{2+\beta}, \cdots$ (we assume throughout this section that $g(x)$ and its derivatives are continuous on $[0, 1]$).

RUTISHAUSER (1963) observed that a modified Romberg method can be used to eliminate the terms in $h^{1/2}, h^{3/2}, h^{5/2}, h^{7/2}, \cdots$ in the error expansion for

$$\int_0^b x^{-1/2} g(x)\,dx,$$

and that a modification of $T(h)$ eliminates the first two terms *before* extrapolation. BULIRSCH (1964) extended this to $\int_0^b x^\beta g(x)\,dx$, with $0 > \beta > -1$.

WATERMAN, YOS and ABODEELY (1964) obtained a generalized Euler–Maclaurin summation formula for $\int_0^1 f(x)\,dx$, where $f(x) = w(x)g(x)$ and $w(x)$ is analytic on $(0, 1]$, using Laplace transforms and contour integration. They confined their attention to the modified trapezium rule ($T(h)$ with $f_0 = 0$), but noted that other formulas can be obtained by linear combination of trapezoidal values. The expansion they obtained for $w(x) = x^\beta$ (with $\mathrm{Re}\,(\beta) > -1$) agreed with Navot's result, and that for $\beta = 0$ reduced to the usual expansion (18). For $w(x) = x^{1/2}e^{-1/x}$, some of the terms in the expansion tend to zero like

$$\exp(-\sqrt{4\pi nk}).$$

MILLER (1968) called this sort of term "uneliminable error" and pointed out that it only affects the estimates with small n (large h).

LYNESS and NINHAM (1967) generalized the results described above to allow more than one singularity and a general quadrature rule:

$$Rf = \sum_{j=0}^{n} w_j R^{[1,\alpha_j]} f. \tag{90}$$

They used generalized function theory to obtain the following error expansion for $f(x) = x^\beta(1-x)^\delta(x)$, where β and δ are not integers and are greater than -1:

$$R^{[n,\alpha]}f - \int_0^1 f(x)\,dx = a_1h^{1+\beta} + a_2h^{1+\delta} + a_3h^{2+\beta} + a_4h^{2+\delta} + \cdots. \tag{91}$$

For $f(x) = x^\beta(1-x)^\delta \ln x\, g(x)$ they obtained the expansion

$$R^{[n,\alpha]}f - \int_0^1 f(x)\,dx = a_1h^{1+\beta}\ln h + a_2h^{1+\beta} + a_3h^{1+\delta} + a_4h^{2+\beta}\ln h + \cdots. \tag{92}$$

(NINHAM (1966) showed how similar expansions could be used in evaluating the "Hadamard finite part" of divergent integrals, with β and/or $\delta < -1$.) In both cases a modified form of Romberg's method can be applied, although the latter case is rather more complicated. When the singularities are inside the interval, the coefficients in the expansion are dependent on h and a modification of Romberg's method is not really a practical proposition. Later NINHAM and LYNESS (1969) investigated the situation where there are singularities in the complex plane near the interval.

HUNTER (1967) suggested that singularities in $\int_a^b w(x)g(x)\,dx$ may be avoided by setting $x = x(t)$, where x is a monotonic function of t such that $x(A) = a$, $x(B) = b$, and $w(x)\,dx = W(t)\,dt$, with $W(t)$ having no singularities in $[A, B]$. For example:

(a) if $a = 0$ and $w(x) = x^{p/q}$, with p and q relatively prime, $q > 1$ and $p + q > 0$, then put $x = t^q$;

(b) if $a = -1$, $b = 1$ and $w(x) = (1-x^2)^{-1/2}$, then $x = \cos t$ leads to $\int_0^\pi g(\cos t)\,dt$ and extrapolation is unnecessary;

(c) if $a = 0$, $b = 1$ and $w(x) = x^{-1/2}(1-x)^{-1/2}$, then put $x = \sin^2 t$.

FOX (1967) showed how Romberg's method can be modified to cope with integrands like $x^{1/2}g(x)$, $x \ln x\, g(x)$, $x^{1/2}\ln x\, g(x)$, $x^{1/2}(1-x)^{1/2}$ and $x^{-1/2}$ (see also MILLER (1968), FOX and MAYERS (1968)). If the integrand is infinite at either

end of the range, $U(h)$ can be used instead of $T(h)$ or $S(h)$. FOX and HAYES (1970) extended the method to integrands like $(1 - x^{1/4})^4$ and observed that *Milne's rule*,

$$M(h) \equiv \tfrac{4}{3}h\{2y_1 - y_2 + 2y_3 + 2y_5 - y_6 + \cdots + 2y_{n-1}\}, \tag{93}$$

can be used instead of $U(h)$. DONNELLY and HAYES (1970) evaluated the Hadamard finite part of divergent integrals, applying extrapolation to approximations obtained from $M(h)$, $U(h)$ and the modified versions of $T(h)$ and $S(h)$ (i.e., those with $f_0 = 0$).

11. Applications of extrapolation processes. Iterative extrapolation has been applied to many problems in recent years. In this section some of these applications are described.

BAUER, RUTISHAUSER and STIEFEL (1963) noted that a modified form of the Romberg process can be used to improve approximate solutions of the ODE (68) obtained by Euler's method (52). In this case the global truncation error "can usually be represented by an asymptotic expansion" of form (1), with $\gamma_j = j$, and the recursion formula for $r_k = 2^{-k}$, $i = 0, 1, 2, \cdots$, and $m = 1, 2, 3, \cdots$, is

$$T_m^i = (2^m T_{m-1}^{i+1} - T_{m-1}^i)/(2^m - 1).$$

The process will converge if $f(x, y)$ is continuous in x and y, and $f(x, y)$ satisfies a Lipschitz condition in y. However, $\sum_{s=i}^{i+m} |c_{i,m,s}|$ can be as large as 8.25. LAURENT (1964b) noted that extrapolation can also be used with Runge–Kutta methods (for which $\gamma_j = j + \delta$, $\delta > 0$) and the *trapezoidal method*:

$$Y_{r+1} = Y_r + \tfrac{1}{2}h\{f(x_{r+1}, Y_{r+1}) + f(x_r, Y_r)\} \tag{94}$$

(for which $\gamma_j = 2j$). DAHLQUIST (1968) recommended using (94) "with repeated Richardson extrapolation and a simple filtering during the first steps," to solve "stiff" systems of ODE's (see also DAHLQUIST (1963a,b)).

RUTISHAUSER (1963) used iterative extrapolation in h^2 to compute values of transcendental functions from recurrence relations (see also HENRICI (1964, p. 242), FILIPPI (1966)) and derivatives from

$$T_0^k \equiv f'(\bar{x}; h_k^2) = (f(\bar{x} + h_k) - f(\bar{x} - h_k))/(2h_k). \tag{95}$$

He noted that in the latter case rounding error can be reduced by using a more slowly decreasing sequence $\{r_k\}$ and modifying the recursion formulas. LAURENT (1964b) investigated extrapolation of symmetric and one-sided initial approximations for total and partial derivatives. FILIPPI (1965b), FILIPPI and ENGELS (1966a,b) and ENGELS (1968a,b) examined error and convergence behavior and considered the use of several different $\{r_k\}$, rational initial approximations and rational extrapolation.

LYNESS and MCHUGH (1963) suggested using extrapolation with a symmetric low order rule (e.g., the product midpoint rule) in multidimensional integration. They tabulated the coefficients α_k for $(h^2, h^4, \cdots)$-extrapolation with $r_k = 1(1 + k)$. LAURENT (1963c, 1964a,b) applied Neville's process to initial approximations obtained from the product rules corresponding to $T(h)$, $U(h)$ and the "compound"

n-point Gauss rule, $r \times G_n$ (see Davis and Rabinowitz (1967, p. 24)). Others to use extrapolation for multidimensional integration were ANDERS (1966), BURGESS (1967), MILLER (1968), HODGSON (1969) and BAKER and HODGSON (1970). LYNESS and MCHUGH (1970) introduced a "concise formalism" so as to obtain the remainder term of the N-dimensional Euler–Maclaurin summation formula (see also SCHÖNHAGE (1970)).

LAURENT (1963b, 1964b) also investigated the application of extrapolation methods to:

(a) BV and EV problems in ODE's—using iterative ("shooting") methods to obtain the initial approximations;

(b) PDE problems—using central differences;

(c) the reduction of variance in Monte Carlo methods;

(d) the solution of IE's—using the trapezium rule (see also MAYERS (1962), LAL and GILLARD (1969), LINZ (1969), WACKER (1969), ATKINSON (1970), BAKER (1971)).

DENNIS (1964) applied variational methods to EV problems in ODE's and obtained approximate solutions with errors of h^4-type (see also GOODWIN (1965)). He used a modified form of Neville's process to carry out the $(h^4, h^6, \cdots)$-extrapolation. ANDERSSEN (1969) used variational methods and extrapolation to solve parabolic PDE's.

12. Asymptotic expansions for differential equations. GRAGG (1964, 1965a,b) was able to show that, when a pth order one-step method is used for the numerical solution of the ODE's (34) under certain conditions of differentiability, the global discretization error at x has the asymptotic expansion (as $h \to 0$ and $n \to \infty$ so that $x = x_0 + nh$ remains fixed)

$$T(h) - a_0 = a_1 h^p + a_2 h^{p+1} + \cdots + a_J h^{p+J-1} + O(h^{p+J}). \tag{96}$$

Here $a_0 = y(x)$ and T and the a_j will depend on x. Equation (96) is of form (1) with $\gamma_j = p + j - 1$ (proved also by WALSTON and WADDELL (1968)), which confirms Henrici's assertion (see §8 (above) and HENRICI (1965)).

When a stable convergent pth order linear multistep method is used, with consistent starting functions having asymptotic expansions in powers of h, to solve the *linear* ODE's

$$\underline{y}' = A(x)\underline{y} + \underline{b}(x), \tag{97}$$

with $\underline{y}(x_0) = \underline{y}_0$, the global discretization error has a "pseudo-asymptotic" expansion of form (96) with the a_j now dependent on h:

$$a_j = a_j(x, h) = \sum_{s=1}^{q} z_s^n u_{s,j}(x), \tag{98}$$

where $z_1, z_2, \cdots, z_q$ are the "essential roots," and the $u_{s,j}(x)$ are independent of h and satisfy certain differential equations. In the case of a nonlinear ODE, the situation is the same for $J < 2p$, but for $J \geqq 2p$ the summation in (98) is over a modified index set. Usually $z_1, z_2, \cdots, z_q$ are the q'th roots of unity (for some $q' \geqq q$), so that $(h^p, h^{p+1}, \cdots)$-extrapolation can be applied for values of

$n_k = (x - x_0)/h_k$ which are divisible by q'. He also showed that a symmetric multistep method will have an asymptotic expansion in powers of h^2 if the starting functions do (see § 14 (below)).

LAURENT (1964b) obtained asymptotic expansions of the form (1) with $J = 2$ for the errors in:

(a) the approximate solution of the ODE (68) by Euler's method (52);

(b) the central difference approximation to $y'' = f(x, y)$ with $y(a) = A$ and $y(b) = B$ (see also KELLER (1968));

(c) the approximate solution of an IE using the trapezoidal rule;

(d) the central difference approximation of Poisson's equation

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = f(x, y)$$

on a square (see also VOLKOV (1965)).

The expansion for (a) has $\gamma_j = j$ and the others have $\gamma_j = 2j$.

STETTER (1965b) extended Gragg's theory to cover IE's, PDE's and BV problems in ODE's. He defined a general discretization, assumed the existence of an asymptotic expansion (with $\gamma_j = p' + j - 1$, $p' > p$) for the *local* discretization error and showed that an asymptotic expansion of form (96) for the *global* discretization error exists if fairly general conditions on stability, convergence and differentiability are satisfied (see also WALSH (1968)). He used his theorem to obtain the coefficients a_j when using Euler's method (52) on $y' = y$, $y_0 = 1$, and when using a central difference method on a second order nonlinear BV problem.

PEREYRA (1965a,b, 1966a,b, 1967a,b, 1968, 1969) modified Stetter's theorem, using general $\{\gamma_j\}$, and presented a generalization of the deferred approach to the limit which he called "the method of successive extrapolations." BULIRSCH (1966) showed that, under certain conditions, the errors in the approximate eigenvector and eigenfunction of a general EV problem will have expansions of form (1) with $\gamma_j = 2j$. HOFMANN (1967) investigated the Dirichlet and Neumann problems of the Laplacian in a square domain and found that the $\{\gamma_j\}$ are determined by the exponents in the expansions of certain quadrature errors involving the boundary value functions. WATT (1967, 1968a,b) restated Stetter's theorem using a new concept of the "inverse" discretization and applied it to a two-step method for solving IV ODE problems.

WERNER (1968) used extrapolation to improve solutions of systems of hyperbolic PDE's obtained by the method of "nebencharacteristics," observed substantial improvement and concluded that "all results confirm the validity of the assumption of the existence of an asymptotic expansion in terms of the discretization parameter." SMITH (1970) investigated the application of extrapolation to hyperbolic PDE's and proved the existence of asymptotic error expansions for Massau's method and a modified midpoint rule, analogous to Gragg's method (see § 14 (below)).

KELLER (1969) showed that, when the "centered difference" method is used to solve the linear ODE's (97), subject to n linear constraints on $[a, b]$, $(h^2, h^4, \cdots, h^{2m})$-extrapolation "can be employed to get high order accuracy approximations with nonuniform nets and piecewise smooth $A(x)$ and $\underline{b}(x)$." Later KELLER (1970) obtained similar results for parabolic PDE's.

13. Polynomial and rational extrapolation. In the previous sections, the extrapolation methods have all been based on (generalized) interpolating polynomials and can be formalized as suggested by BULIRSCH and STOER (1964, 1965): for an approximation $T(h)$ having an asymptotic error expansion of form (1) with $J \geqq m$, we define the (generalized) polynomial

$$\hat{T}^i_m(h) \equiv b_0 + b_1 h^{\gamma_1} + b_2 h^{\gamma_2} + \cdots + b_m h^{\gamma_m}, \tag{99}$$

by imposing the conditions

$$\hat{T}^i_m(h_k) = T(h_k), \qquad k = i, i+1, \cdots, i+m. \tag{100}$$

$T(0)$ is approximated by $\hat{T}^i_m(0) = b_0$ and we define

$$T^i_m \equiv T(h_i, h_{i+1}, \cdots, h_{i+m}) \equiv b_0.$$

Constructing a linear operator L^i_m from

$$\begin{aligned} &L^i_m T = \sum_{s=i}^{i+m} c_{i,m,s}\, T(h_s), \qquad L^i_m 1 = 1, \\ &L^i_m h^{\gamma_j} = 0, \qquad\qquad\qquad\qquad j = 1, 2, \cdots, m, \end{aligned} \tag{101}$$

and applying it to (99), we obtain

$$\begin{aligned} L^i_m \hat{T}^i_m &= L^i_m\left(b_0 + \sum_{j=1}^{m} b_j h^{\gamma_j}\right) \\ &= b_0(L^i_m 1) + \sum_{j=1}^{m} b_j (L^i_m h^{\gamma_j}), \end{aligned}$$

so

$$L^i_m\, \hat{T}^i_m = T^i_m.$$

In the case $\gamma_j = j\gamma$, Bulirsch and Stoer generalized (86) to:

$$T^i_m = \frac{h_i^{\gamma}\, T^{i+1}_{m-1} - h^{\gamma}_{i+m} T^i_{m-1}}{h_i^{\gamma} - h^{\gamma}_{i+m}} \tag{102}$$

or

$$T^i_m = T^{i+1}_{m-1} + \frac{T^{i+1}_{m-1} - T^i_{m-1}}{(h_i/h_{i+m})^{\gamma} - 1},$$

i.e., Neville's process extrapolation of $\{F(h_k^{\gamma}) = T(h_k)\}$ to $F(0)$. Unless $\{r_k\}$ is restricted there is no such simple formula available when $\{\gamma_j\}$ is arbitrary. However, for $r_k = \rho^k$, with $0 < \rho < 1$, they obtained

$$T^i_m = (T^{i+1}_{m-1} - \rho^{\gamma_m} T^i_{m-1})/(1 - \rho^{\gamma_m}) \tag{103}$$

or

$$T^i_m = T^{i+1}_{m-1} + (T^{i+1}_{m-1} - T^i_{m-1})/(\rho^{-\gamma_m} - 1).$$

They derived an error bound for $|T^i_m - T(0)|$ when $r_{k+1}/r_k \leqq \rho < 1$ and $\gamma_{j+1} - \gamma_j \geqq \gamma > 0$ and deduced that, if an error expansion of form (1) is not

possible for J greater than some J_0, then the error in $T_m^i \to 0$ like $h_i^{\gamma m+1}$ for $m \leqq J_0$ and like $h_i^{\gamma J_0+1}$ for $m \geqq J_0$. Thus there is little to be gained by computing more than J_0 columns. They proved that, if $\lim_{i\to\infty} T_0^i = T(0)$ and *either* $\gamma_j = j\gamma$ and $r_{k+1}/r_k \leqq \rho < 1$ for all k *or* $r_k = \rho^k$ and $\sum_{j=0}^{\infty} \rho^{\gamma j}$ is convergent, then

$$\lim_{m\to\infty} T_m^i = T(0).$$

Then they suggested that, when $\gamma_j = j\gamma$, *rational extrapolation* as developed by STOER (1961) could be used instead of polynomial extrapolation. In this case $T(0)$ is approximated by $T_{\mu,\nu}^i \equiv \hat{T}_{\mu,\nu}^i(0)$, where

$$\begin{aligned} &\hat{T}_{\mu,\nu}^i(h) \equiv P_{\mu,\nu}^i(h)/Q_{\mu,\nu}^i(h), \\ &P_{\mu,\nu}^i(h) \equiv \sum_{j=0}^{\mu} p_j h^{j\gamma}, \qquad Q_{\mu,\nu}^i(h) \equiv \sum_{j=0}^{\nu} q_j h^{j\gamma}, \\ &\hat{T}_{\mu,\nu}^i(h_k) = T(h_k), \qquad\qquad k = i, i+1, \cdots, i+\mu+\nu \end{aligned} \tag{104}$$

(note that when $\nu = 0$, we have polynomial extrapolation). The recursion formulas analogous to (102) are rather complicated but they can be simplified by choosing $\mu = [m/2]$ and $\nu = m - [m/2]$ and writing $T_{\mu,\nu}^i = T_m^i$. In this case the formulas are

$$\begin{aligned} T_{-1}^i &= 0, && i \geqq 1, \\ T_0^i &= T(h_i), && i \geqq 1, \\ T_m^i &= \frac{h_i^\gamma \Theta_m^i T_{m-1}^{i+1} - h_{i+m}^\gamma T_{m-1}^i}{h_i^\gamma \Theta_m^i - h_{i+m}^\gamma}, && m \geqq 1, \end{aligned} \tag{105}$$

or

$$T_m^i = T_{m-1}^{i+1} + \frac{T_{m-1}^{i+1} - T_{m-1}^i}{(h_i/h_{i+m})^\gamma \Theta_m^i - 1},$$

where

$$\Theta_m^i = \frac{T_{m-1}^i - T_{m-2}^{i+1}}{T_{m-1}^{i+1} - T_{m-2}^{i+1}}.$$

There is an obvious analogy with (102), but unlike all previous formulas, the transformation in this case is *nonlinear*.

They proved that, under certain conditions, when this method is applied to quadrature using trapezoidal values in the first column,

$$T_{\mu,\nu}^i - \int_0^1 f(x)\,dx = (-)^\nu h_i^2 h_{i+1}^2 \cdots h_{i+m}^2 \beta_{\mu+1} f^{(2\mu+2)}(\xi) q_\nu/q_0 \tag{106}$$

with $0 \leqq \xi \leqq 1$ (compare (87)). Tests using $\{r_k\} = Q$ for quadrature indicated that $\{T_{\mu,\nu}^0; \mu = [m/2], \nu = m - [m/2]\}$ converges quicker than $\{T_{m,0}^0\}$ or $\{T_{0,m}^0\}$ (see also KAPFER (1966)), but later BULIRSCH and STOER (1967b) observed that, because the algorithm is more complicated, "this advantage is not necessarily reflected by the computing time needed." When (105) was compared with (102) as a method

of improving approximate solutions of $y' = y$, $y_0 = 1$, using Euler's method with $h_k = 2^{-k}$, it was found to require fewer evaluations to attain a specified accuracy. FILIPPI and ENGELS (1966a) applied rational extrapolation to numerical differentiation.

14. Gragg's method. When GRAGG (1964, 1965a,b) obtained his results about asymptotic error expansions for symmetric multistep methods (see § 12 (above)) he observed that knowledge about the derivatives of $f(x, y)$ is usually required in order to obtain suitable starting functions, but that in two cases nothing besides the starting value y_0 is needed. The first case is that of the *trapezoidal method*, but unless we can solve the implicit difference equation (94) exactly at each step, the expansion is restricted in length.

The second case is that of the *midpoint method* (35). If $Y_0 = y_0$ and $Y_1 = y_0 + hf(x_0, y_0)$ are used as starting values, the error has a "pseudo-asymptotic" expansion (as $h \to 0$ and $n \to \infty$ so that $x = x_0 + nh$ remains fixed):

$$T(h) - a_0 = a_1h^2 + a_2h^4 + \cdots + a_Jh^{2J} + O(h^{2J+2}),$$

where

$$T(h) = Y_n, \qquad a_0 = y(x),$$

and

$$a_j = a_j(x, h) = u_j(x) + (-)^n v_j(x), \tag{107}$$

with $u_j(x)$ and $v_j(x)$ independent of h. In this case extrapolation in h^2 can be applied with a sequence $\{h_k\}$ such that $n_k = (x - x_0)/h_k$ is either even for all k or odd for all k.

Gragg suggested modifying the midpoint method in order to obtain two approximate solutions analogous to (11) and (23). Using $Y_0 = y_0$ and $Z_0 = y_0 + \frac{1}{2}hf(x_0, y_0)$ as starting values, we compute

$$Y_{r+1} = Y_r + hf(x_r + \tfrac{1}{2}h, Z_r), \qquad Z_{r+1} = Z_r + hf(x_r + h, Y_{r+1}) \tag{108}$$

for $r = 0, 1, \cdots, n - 1$, and we define $U(h)$ and $T(h)$ by

$$U(h) \equiv Y_n, \quad \text{and} \quad T(h) \equiv Z_n - \tfrac{1}{2}hf(x, Y_n). \tag{109}$$

If $f(x, y)$ is independent of y, these reduce to (11) and (23). Finally $G(h)$ is defined by

$$G(h) \equiv (U(h) + T(h))/2. \tag{110}$$

U, T and G all have error expansions of the h^2-type with coefficients independent of h, so extrapolation in h^2 can be applied with *any* sequence $\{h_k\}$. Note that U, T and G are all functions of x as well as h. This can be emphasized by writing $G(x; h)$ etc.

A "step-by-step" algorithm using extrapolation of the *modified midpoint method* (110) to integrate an ODE (or system of ODE's) from $x = a$ to $x = b$ can be based on the following:

(a) choose a "global" step H, such that $(b - a)/H$ is integral, and a sequence $\{h_0, h_1, \cdots, h_m\}$ such that H/h_k is integral for $k = 0, 1, \cdots, m$;
(b) set $x_0 = a, y_0 = y(a)$ and $x = a + H$;
(c) use (110) to obtain $\{T_0^k = G(a + H; h_k)\}$;
(d) use (102) or (105) with $\gamma = 2$ to obtain $T_m^0 = G(a + H; h_0, h_1, \cdots, h_m)$;
(e) set $x_0 = a + H, y_0 = T_m^0$ and $x = a + 2H$;
(f) use (110) and (102) or (105) to obtain $G(a + 2H; h_0, h_1, \cdots, h_m)$, etc.

Gragg observed that "this entire process is a Runge–Kutta (one-step) method" which "guarantees the numerical stability (as $h \to 0$) of the step-by-step algorithm." He also developed a similar method for solving the second order ODE (69).

Gragg pointed out that in G the leading unstable component of the discretization error has been eliminated, from which STETTER (1968b) deduced that G is always "asymptotically strongly stable." Stetter also noted that the extrapolation process has a stabilizing effect since the solutions computed with the largest h_k have the least weight in the extrapolated value. Later STETTER (1969) investigated the stability of the entire process and concluded that while the stability region is not very large, this is nevertheless an improvement on the basic midpoint method "the absolute stability region of which is empty." In papers to be published, STETTER (1970) examines general symmetric linear two-step schemes and BUTCHER (1970) mentions "a characterization ... for Runge–Kutta methods which for appropriately smooth functions have a global truncation error with asymptotic expansions in even powers of the step size."

Gragg compared the *Gragg–Neville method* (using (110) and (102) as above with $m = 6$ or 7) and the *Gragg–Stoer method* ((110) and (105) with $m = 6$ or 7) with a Runge–Kutta 4th order method and the Adams predictor-corrector pairs of order 4, 5 and 6. BULIRSCH and STOER (1966a) carried out similar tests and observed that the Gragg–Stoer method obtained a specified accuracy with fewer function evaluations (see also CLARK (1968) and SKAPPEL (1969)). They suggested including an automatic step size correction.

15. Modifications of Romberg's method. Several suggestions have been made recently concerning possible improvements and generalizations of Romberg's method. Some of these are described in this section.

LAURENT (1963c, 1964a,b) observed that extrapolation can be applied to initial approximations obtained from composite Gauss rules. For instance, we can use the composite $(p + 1)$-point rule, which is exact for polynomials of degree $2p + 1$, and set up a triangular scheme of approximations to $\int_0^1 f(x)\,dx$ with

$$
\begin{aligned}
&G_m^i = 0, && m < p,\\
&G_p^i = (n_i \times G_{p+1})f, &&\\
&G_m^i = (4^m G_{m-1}^{i+1} - G_{m-1}^i)/(4^m - 1), && m > p,
\end{aligned}
\tag{111}
$$

where $n_i = 2^i \times n$ and $i \geqq 0$. Laurent noted that this "Gauss–Romberg" method combines the precision and economy of Gaussian formulas with the simplicity of iterative extrapolation (see also LYNESS (1970b)).

MEIR and SHARMA (1965) suggested using higher order Newton–Cotes formulas to obtain the initial approximations. In particular, using Simpson's rule

with $h_k = 1/(2 + 2k)$, they obtained the following expression for E_S, the error in S_m^0:

$$E_S \equiv S_m^0 - \int_0^1 f(x)\,dx = c_m \beta_{m+1} f^{(2m+2)}(\xi_S), \tag{112}$$

where

$$c_m = \frac{2 - 2^{-2m+1}}{m(m+1)(2m+1)(m!)^2},$$

and $0 \leqq \xi_S \leqq 1$ (note that $S_0^i = 0$, $S_1^i = S(h_i)$, conforming with (111)). Comparing (112) with

$$E_T \equiv T_m^0 - \int_0^1 f(x)\,dx = \frac{\beta_{m+1} f^{(2m+2)}(\xi_T)}{((m+1)!)^2}, \tag{113}$$

where $0 \leqq \xi_T \leqq 1$ and $h_k = 1/(1 + k)$ (see (87)), they observed that

$$\frac{E_S}{E_T} \sim \frac{(2 - 2^{-2m+1})(m+1)}{m(2m+1)} \sim \frac{1}{m} \tag{114}$$

and concluded that the decrease in error and in number of extrapolations more than compensated for the increase in function evaluations (see also TURNBULL (1967), MANOHAR and TURNBULL (1968)).

ELSNER (1966) showed how extrapolation of Newton–Cotes values can be carried out in an elegant fashion. If $C(h)$ is a Newton–Cotes composite rule of "polynomial degree" $2p + 1$, the polynomial $\hat{C}_{p+m}^i(h)$ is defined by

$$\begin{aligned} &\hat{C}_{p+m}^i(h) \equiv b_0 + b_1 h^{2p+2} + b_2 h^{2p+4} + \cdots + b_m h^{2p+2m}, \\ &\hat{C}_{p+m}^i(h_k) = C(h_k), \qquad\qquad k = i, i+1, \cdots, i+m. \end{aligned} \tag{115}$$

Then the operator L_m^i, defined by (101) with $\gamma_j = 2j$, can be applied to

$$\hat{A}_m^i(h) \equiv h^{-2p} \hat{C}_m^i(h), \tag{116}$$

yielding

$$A_m^i \equiv L_m^i \hat{A}_m^i = L_m^i(b_0 h^{-2p}) + \sum_{j=1}^{m} L_m^i(b_j h^{2j}).$$

Hence

$$C_{p+m}^i = A_m^i / P_m^i, \tag{117}$$

where

$$P_m^i \equiv L_m^i(h^{-2p}) \tag{118}$$

and

$$C_{p+m}^i \equiv \hat{C}_{p+m}^i(0) = b_0$$

(see also SCHMIDT (1968), MILLER (1968), LYNESS (1970b)). A_m^i and P_m^i can be computed by recursion formula (102).

Comparing the methods based on $T(h)$ and $S(h)$ ($p = 0$ and 1 respectively) Elsner noted that, when $\{r_k\} = Q$ is used, T_m^0 is of order 2 higher than S_{m-1}^0 for very nearly the same number of function evaluations. He concluded that it will generally be better to use $T(h)$, since the work involved in the extra extrapolations is usually negligible in comparison. ROBINSON (1969) experimented with a "Romberg–Weddle" method in which the initial approximations are obtained from (15). Romberg-type methods based on general quadrature rules were investigated by BAKER (1969), HODGSON (1969), BAKER and HODGSON (1970) and LYNESS (1970b).

KRASUN and PRAGER (1965) observed that rounding errors in Romberg's method could be reduced by forming a "skeleton table." In this table, the U_m^i are obtained in the usual way (see Table 8), the T_m^0 for $m > 0$ are obtained from (76), the T_m^i for $i > 0$ are *not* computed for m less than some M, and the T_M^i are obtained from (62); thus (60) is not used at all (see also FAIRWEATHER (1969)).

PRAGER (1965) suggested an "adaptive" Romberg method for computing $\int_a^b f(x)\,dx$ (see also ELLIOT and PRAGER (1965), DAVIS and RABINOWITZ (1967)). The sequence $\{r_k = 2^{-k}\}$ is used and the convergence criterion is based on the quantities

$$D_m \equiv |T_{m-1}^0 - T_m^0|, \qquad m = 1, 2, 3, 4. \tag{119}$$

The method proceeds as follows:

(a) Choose $h(= h_0$, say) and a tolerance ε.

(b) Compute T_0^0 and T_1^0 for $\int_a^{a+h} f(x)\,dx$.

(c) If $D_1 < \varepsilon$, accept T_1^0 and increase h to $1.5h$; otherwise compute T_2^0 and if $D_2 < \varepsilon$, accept T_2^0 and leave h unaltered; otherwise compute T_3^0 and if $D_3 < \varepsilon$, accept T_3^0 and reduce h to $0.6h$; otherwise compute T_4^0 and if $D_4 < \varepsilon$, accept T_4^0 and reduce h to $0.6h$.

(d) If D_m was less than ε for $m = 1, 2, 3$ or 4, proceed with the next interval; otherwise reduce h to $0.6h$ and attempt the integration over $[a, a + 0.6h]$, etc. The last interval may have to be adjusted in order to conclude at b. If more than, say, $8(b - a)/h_0$ steps have been taken without reaching b, an "error exit" is made.

RABINOWITZ (1966) compared this adaptive routine with the usual Romberg method and the *adaptive Simpson method* (McKeeman (1962, 1963a, b), McKeeman and Tesler (1963)) and concluded that it "requires more information to be given by the user and appears to be less efficient." Adaptive Romberg methods have also been investigated by MILLER and BURKE (1969), MILLER (1970) and DE BOOR (1970a, b). O'HARA and SMITH (1969) used the 9-point Romberg method in combination with Boole's rule (14) and two 7-point Clenshaw–Curtis quadratures (Clenshaw and Curtis (1960)) in an adaptive algorithm.

HAVIE (1967) observed that the cosine transformation, applied by Smith (1965) to the modified Simpson rule, can be used with Romberg's method in the evaluation of $\int_{-1}^{+1} f(x)\,dx$, by defining

$$T_1^i \equiv h_i \sum_{r=1}^{N} f(\cos(rh_i)) \sin(rh_i) + \frac{h_i^2}{12}(f(1) + f(-1)) \tag{120}$$

and

$$U_1^i \equiv h_i \sum_{r=1}^{N} f(\cos((r-\tfrac{1}{2})h_i)) \sin((r-\tfrac{1}{2})h_i) - \frac{h_i^2}{24}(f(1)+f(-1)), \tag{121}$$

where $h_i = \pi/2^i$. T_m^i and U_m^i for $m > 1$ can be computed from (60), (61) and (62). Havie noted that this algorithm will have an advantage "when dealing with integrals where the integrands behave in a nonpolynomial way towards the ends of the integration intervals," gave examples which supported this (see also HAVIE (1969b)) and indicated how the number of evaluations of sine and cosine can be kept to a minimum. He also suggested that the way in which the Romberg algorithm is applied can be modified (as suggested by Jagermann (1966) for the midpoint rule) in order to avoid undesired effects due to the weight function $w(x)$ in an integral of the form $\int_a^b w(x)g(x)\,dx$.

LYNESS (1967, 1970a) and LYNESS and MOLER (1969) pointed out that when the equations

$$T(h_k) = b_0 + b_1 h_k^2 + b_2 h_k^4 + \cdots + b_m h_k^{2m}, \qquad k = i, i+1, \cdots, i+m, \tag{122}$$

are solved in order to obtain $T_m^i (= b_0)$ as an approximation to $I_0 = \int_0^1 f(x)\,dx$, the values of $b_1, b_2, \cdots, b_m$ can also be computed as approximations to

$$a_j = (-)^{j-1}\beta_j(f^{(2j-1)}(1) - f^{(2j-1)}(0)), \qquad j = 1, 2, \cdots, m \tag{123}$$

(the a_j can be used in computing Fourier coefficients for $f(x)$). $T_{i,m,j} (= b_j)$ is computed by the "generalized Romberg method," as follows:

$$\begin{aligned} T_{i,m,j} &= 0, \qquad j < 0 \quad \text{or} \quad j > m, \\ T_{i,0,0} &= T(h_i), \qquad i \geqq 0, \end{aligned} \tag{124}$$

and

$$T_{i,m,j} = \frac{(h_i^2 T_{i+1,m-1,j} - h_{i+m}^2 T_{i,m-1,j}) - (T_{i+1,m-1,j-1} - T_{i,m-1,j-1})}{h_i^2 - h_{i+m}^2}, \tag{125}$$

$j = 0, 1, 2, \cdots, m$, and $m \geqq 1$ (compare (74) and note that, when $j = 0$, (125) reduces to (86), since $T_{i,m,0} \equiv T_m^i$).

Lyness and Moler also investigated the use of the midpoint rule (23), the *alternating trapezoidal sum*,

$$R^{[2n,1]}(f(x)\cos 2\pi n x) \equiv \tfrac{1}{2}(R^{[n,1]}f(x) - R^{[n,0]}f(x)), \tag{126}$$

and the *alternating rectangular sum*,

$$R^{[2n,0]}(f(x)\sin 2\pi n x) \equiv \tfrac{1}{2}(R^{[n,-1/2]}f(x) - R^{[n,0]}f(x)) \tag{127}$$

(where $R^{[n,\alpha]}f(x)$ is defined by (89)) for computing the initial approximations (when (126) and (127) are used, some adjustments are necessary), and obtained generalizations of the results of § 9 (above). LYNESS (1968b) noted that (125) can also be applied to the calculation of Stieltjes-type integrals.

LYNESS and DELVES (1967) observed that the error expansion for $T(h)$ has terms in $h^2, h^6, h^{10}, \cdots$ for contour integration round a square, $h^2, h^4, h^8, h^{10}, h^{14}, \cdots$ for contour integration round a triangle or hexagon, and $h^4, h^8, h^{12}, \cdots$ for the

integral over a square of a harmonic function of two variables (see also MILLER (1968)). They suggested the introduction of a "noneliminating" step (when $r_k = \rho^k$): if h^{2m} does not need to be eliminated, put $T_m^i = T_{m-1}^i$. For integration round a square, the scheme in Table 9 is obtained with $T_2^i = T_1^i$, $T_4^i = T_3^i$.

TABLE 9

$$\begin{array}{cccccc} T_0^0 & & & & & \\ T_0^1 & T_1^0 & T_2^0 & & & \\ T_0^2 & T_1^1 & T_1^1 & T_3^0 & T_4^0 & \\ T_0^3 & T_1^2 & T_2^2 & T_3^1 & T_4^1 & T_5^0 \end{array}$$

The expression they obtained for the truncation error with $r_k = 2^{-k}$ reduces to (18) if all the steps are noneliminating and to (85) if they are all eliminating.

16. Error estimates and asymptotic bounds. Relations like (85) and (87), which express the error in an approximation in terms of the value of a derivative at an unknown point, are not usually very helpful in practical computation, although they can be used to compare the theoretical accuracy of different approximations (as can the error bounds investigated by MARSAL (1965), STROUD (1965, 1966), MEINGUET (1966) and BAKER (1968)). Various techniques for obtaining "asymptotic" bounds (or estimates) for the error, which have been developed in recent years, are reviewed in this section.

ROMBERG (1955) used Taylor series expansions to show that T_m^i and U_m^i may bracket the true value of the integral (see § 7 (above)) and BAUER (1961a) obtained conditions under which this will be true for $i = 0$ (see § 9 (above)). However, little use was made of this property until KUBIK (1965) produced an algorithm based on theoretical results obtained by HAVIE (1966, 1967), who deduced from the Euler–Maclaurin formula (18) and the second Euler formula (25) that, "under rather general conditions ... the errors of T_m^i and U_m^i are of opposite sign" in which case

$$|T_m^{i+1} - I| = \left| \frac{T_m^i + U_m^i}{2} - I \right| \leqq \frac{|T_m^i - I| + |U_m^i - I|}{2},$$

i.e.

$$|T_m^{i+1} - I| \leqq |T_m^i - U_m^i|/2. \tag{128}$$

Thus, if the table is built up as Romberg suggested (see Table 8), error estimates are obtained with very little additional calculation. However, Havie gave two examples where T_m^i and U_m^i do not bracket the true result in the early part of the table (i.e., when $i + m$ is small). He observed that the U-scheme should have slightly faster convergence and "seems more advantageous when $f(a) = 0/0$," and that the failure of Romberg's method to improve the convergence of the trapezoidal values for integrals like $\int_0^\infty e^{-x^2}\,dx$ is shown up by the monotonic increase of $|T_j^{m-j} - U_j^{m-j}|$ for $j = 0, 1, \cdots, m$ (i.e., along the rows).

STROM (1967) observed that Havie's results can be used to show that

$$|(3T_m^{i+1} - T_m^i)/2 - I| \leqq |T_m^{i+1} - T_m^i|/2 \tag{129}$$

(proved, for $m = 1$, by DAHLQUIST (1966)). He then proved that, if $f^{(2m+2)}(x) \geqq 0$ in $[0, 1]$, then $2T_m^{i+1} - T_m^i (= U_m^i)$ is "the largest lower bound (for $I = \int_0^1 f(x)\,dx$) that can be obtained from the elements T_m^{i+1} and T_m^i under the sole assumption on the sign of $f^{(2m+2)}(x)$ in $[0, 1]$." He suggested using automatically constructed "majorants" to bound the error in $(3T_m^{i+1} - T_m^i)/2$.

Later HAVIE (1969a) expressed the errors in T_m^i and U_m^i in terms of Bernoulli polynomials and their related periodic functions, obtaining (85) and

$$U_m^i - \int_0^1 f(x)\,dx = \frac{-\omega\beta_{m+1} f^{(2m+2)}(\eta)}{2^{(m+2i)(m+1)}}, \tag{130}$$

where $\omega = 1 - 2^{-(2m+1)}$ and $0 \leqq \eta \leqq 1$ (compare (25) and (85)). He deduced that, if $f^{(2m+2)}$ is continuous in $[0, 1]$ and if $f^{(2m+1)}(1) \neq f^{(2m+1)}(0)$, then, for increasing values of i, the errors in T_m^i and U_m^i will get the opposite sign. Observing that $|T_m^i - U_m^i|/2$ may greatly overestimate the error in T_m^{i+1}, he suggested using the asymptotic error estimate

$$T_m^{i+1} - I \sim E_m^{i+1} \equiv \frac{(T_m^i - U_m^i)}{2(4^{m+1} - 1)}, \tag{131}$$

with the closeness to unity of

$$R_m^{i+1} \equiv 4^{m+1} E_m^{i+1} / E_m^i \tag{132}$$

as a measure of the quality of the estimate. LYNCH (1965, 1967) had proposed using

$$E_m^{i+1} \equiv (T_m^i - T_m^{i+1})/(4^{m+1} - 1) \tag{133}$$

with (132). From (62) we can deduce that

$$(T_m^i - T_m^{i+1}) = T_m^i - (T_m^i + U_m^i)/2 = (T_m^i - U_m^i)/2,$$

so the two estimates are identical. DE BOOR (1970a,b) used (132) and (133) in an adaptive quadrature algorithm.

BULIRSCH and STOER (1965, 1966b, 1967a) showed that, when polynomial or rational extrapolation is applied to any approximation, $T(h)$, having an error expansion of form (1) with $\gamma_j = j\gamma$, the extrapolants satisfy

$$T_m^i - T(0) = h_i^\gamma h_{i+1}^\gamma \cdots h_{i+m}^\gamma (c_{m+1} + O(h_i^\gamma)). \tag{134}$$

They used this result to demonstrate that, if $\bar{U}_m^i$ is defined by

$$\bar{U}_m^i = (1 + \alpha) T_m^{i+1} - \alpha T_m^i, \tag{135}$$

with

$$\alpha = 1 + \frac{2}{(h_i/h_{i+m+1})^\gamma - 1}, \tag{136}$$

and if $c_{m+1} \neq 0$, then for fixed m,

$$\lim_{i \to \infty} \frac{T_m^i - T(0)}{\bar{U}_m^i - T(0)} = -1, \tag{137}$$

and so, for i greater than some i_0, T_m^i and $\bar{U}_m^i$ tend monotonically from opposite sides to the exact result, $T(0)$. They noted that T_m^i and $\bar{U}_m^i$ are more likely to be upper and lower bounds of $T(0)$ than T_m^{i+1} and V_m^{i+1}, where

$$V_m^{i+1} \equiv \alpha T_m^{i+1} - (\alpha - 1)T_m^i \tag{138}$$

(NEUMANN (1966) used V_m^1 to show that, under certain conditions,

$$|T_{m+1}^0 - T(0)| \leqq |T_{m+1}^0 - T_m^1|).$$

For arbitrary $\{\gamma_j\}$ and $r_k = \rho^k$, $0 < \rho < 1$, the above result (137) will hold for polynomial extrapolation, i.e., T_m^i and $\bar{U}_m^i$ will be *asymptotic upper and lower bounds*, if

$$\alpha = 1 + 2/(\rho^{-\gamma_{m+1}} - 1). \tag{139}$$

In this case, if $\tilde{U}_m^i$ is defined by

$$\tilde{U}_m^i = 2T_m^{i+1} - T_m^i, \tag{140}$$

it can be regarded as the result of applying polynomial extrapolation to

$$\tilde{U}(h) = 2T(\rho h) - T(h),$$

and for quadrature, with $\rho = \frac{1}{2}$, we have the U-scheme of Romberg's method.

Bulirsch and Stoer showed how to obtain upper and lower bounds for:

(a) the value of an integral, using rational extrapolation of trapezoidal values (see also BULIRSCH and RUTISHAUSER (1968));

(b) the solution of an IV problem in ODE's, using the Gragg–Stoer method; and

(c) the EV of an ODE, using central differences and polynomial extrapolation (see also BULIRSCH (1966)).

They noted that it is very difficult to say how large i must be in order to ensure that T_m^i and $\bar{U}_m^i$ are upper and lower bounds, and suggested that, for practical purposes, the extrapolation should be stopped "if a finite number of T_m^i and $\bar{U}_m^i$ decrease or increase monotonically and if $|T_m^i - \bar{U}_m^i|$ is small enough" (this was used by BULIRSCH and STOER (1967b) for quadrature).

SCHMIDT (1966) showed that for sufficiently large i, $T(0)$ will lie between T_m^i and $\bar{T}_m^i$ and also between T_m^i and $\tilde{T}_m^i$, where

$$\begin{aligned} \bar{T}_m^i &= T_{m-1}^{i+1} + (T_{m-1}^{i+1} - T_m^i)/(\Omega_m^i - 1), \\ \tilde{T}_m^i &= T_{m-1}^{i+1} + (T_{m-1}^{i+1} - T_m^i)/(\Omega_m^{i+1} - 1), \\ \Omega_m^i &= (T_m^i - T_m^{i-1})/(T_{m-1}^{i+1} - T_{m-1}^i), \end{aligned} \tag{141}$$

and the $\{T_m^i\}$ are obtained by polynomial extrapolation, with *either* $\gamma_j = j\gamma$ and $r_{k+1}/r_k \leqq \rho < 1$ *or* arbitrary $\{\gamma_j\}$ and $r_k = \rho^k$.

He also obtained analogous results for the *ε-algorithm* (see, for example, WYNN (1956a, 1963), BAUER (1965)), which is based on the assumption of an asymptotic expansion, for an approximation x_i of a quantity z, of the form

$$x_i = z + c_1\lambda_1^i + c_2\lambda_2^i + \cdots + c_J\lambda_J^i + o(\lambda_J^i) \tag{142}$$

(KAHANER (1969) and DE BOOR (1970b) observed that the ε-algorithm can be used to solve (1) for a_0 when the γ_j are unknown and $h_k = \rho^k h$). The ε-algorithm computes the quantities ε_m^i, with $i \geqq 0$, from

$$\begin{aligned} &\varepsilon_{-1}^i = 0, \qquad \varepsilon_0^i = x_i, \\ &\varepsilon_m^i = \varepsilon_{m-2}^{i+1} + 1/(\varepsilon_{m-1}^{i+1} - \varepsilon_{m-1}^i) \end{aligned} \tag{143}$$

(only the $\{\varepsilon_{2m}^i\}$ are improvements). In particular,

$$\varepsilon_2^i = \varepsilon_0^{i+1} + 1/(\varepsilon_1^{i+1} - \varepsilon_1^i),$$

and, after substituting for ε_1^{i+1} and ε_1^i, we obtain the "δ^2-process" of AITKEN (1926):

$$\varepsilon_2^i = x_{i+1} - \frac{(x_{i+1} - x_i)^2}{x_{i+1} - 2x_i + x_{i-1}} \tag{144}$$

(see also OVERHOLT (1965, 1968), who discussed "Richardson-like" techniques).

Later SCHMIDT (1968) showed that, when $\gamma_j = j\gamma + \delta$ and $r_{k+1}/r_k \leqq \rho < 1$, iterative extrapolation can be carried out according to

$$\begin{aligned} &T_0^i = T(h_i), \qquad H_0^i = h_i^{-\delta}, \\ &T_m^i = T_{m-1}^{i+1} + \frac{T_{m-1}^{i+1} - T_{m-1}^i}{D_m^i - 1}, && m \geqq 1, \\ &H_m^i = H_{m-1}^{i+1} + \frac{H_{m-1}^{i+1} - H_{m-1}^i}{(h_i/h_{i+m})^\gamma - 1}, && m \geqq 1, \end{aligned} \tag{145}$$

where

$$D_m^i = h_i^\gamma H_{m-1}^{i+1}/(h_{i+m}^\gamma H_{m-1}^i)$$

(note that if $\delta = 0$, then $H_m^i \equiv 1$ and (145) reduces to (102)). In this case, $\bar{U}_m^i$, defined by (135) with

$$\alpha = 1 + 2/(D_{m+1}^i - 1),$$

and T_m^i are asymptotic upper and lower bounds; i.e., for sufficiently large i,

$$|(T_m^i + \bar{U}_m^i)/2 - T(0)| \leqq |T_m^i - \bar{U}_m^i|/2. \tag{146}$$

Schmidt observed that

$$T_{m+1}^i = (T_m^i + \bar{U}_m^i)/2$$

and hence

$$|T_{m+1}^i - T(0)| \leqq |T_{m+1}^i - T_m^i|. \tag{147}$$

ENGELS (1968a) investigated enclosing formulas for numerical differentiation, approximating $f'(\bar{x})$, for example, by

$$T_0^i = (f(\bar{x} + h_i) - f(\bar{x} - h_i))/(2h_i),$$

setting

$$\bar{U}_0^i = (1 + \alpha)T_0^i - \alpha(f(\bar{x} + \beta h_i) - f(\bar{x} - \beta h_i))/(2\beta h_i) \tag{148}$$

and using polynomial extrapolation to obtain T_m^i and $\bar{U}_m^i$, which will enclose $f'(\bar{x})$ if $\alpha = 2/(\beta^2 - 1)$ and the higher derivatives are sufficiently small.

17. Two generalizations of Neville's process. LARKIN (1967a) generalized Neville's process to include rational interpolation, using three formulas:

(a) the "triangle rule" for polynomial interpolation:

$$f_{i,m} = \frac{(\bar{x} - x_i)f_{i+1,m-1} - (\bar{x} - x_{i+m})f_{i,m-1}}{x_{i+m} - x_i} \tag{149}$$

(compare (86)), which is Neville's process;

(b) the "triangle rule" for reciprocal-polynomial interpolation:

$$f_{i,m} = \frac{x_{i+m} = x_i}{(\bar{x} - x_i)/f_{i+1,m-1} - (\bar{x} - x_{i+m})/f_{i,m-1}}; \tag{150}$$

(c) the "rhombus rule" for rational interpolation:

$$f_{i,m} = f_{i+1,m-2} + \frac{x_{i+m} - x_i}{(\bar{x} - x_i)/(f_{i+1,m-1} - f_{i+1,m-2}) - (\bar{x} - x_{i+m})/(f_{i,m-1} - f_{i+1,m-2})} \tag{151}$$

(compare (105)).

Larkin suggested two algorithms: A_i, which uses (149) for the first i columns and then (151), and B_i, which uses (150) for the first i columns and then (151). It is thus possible to choose an algorithm to provide a rational interpolating function with numerator and denominator of specified degrees. He noted that algorithms suggested by WYNN (1956c, 1960) and STOER (1961) are included as special cases. In a later paper, LARKIN (1967b) generalized Neville's process even further, developing a process for constructing polynomial and nonpolynomial interpolating functions by means of simple recurrence relations. Special cases include polynomials, reciprocal polynomials, rational functions and trigonometric series (also investigated by HUNTER (1968)).

MILLER (1968) showed that Neville's process can be viewed as "a process for term-by-term elimination of error, expressed as a power series," and introduced a matrix formulation based on the Taylor series expansion of $f(x_i)$ about $\bar{x}$. He applied the process to integration (in one and two dimensions) and summation of series and showed how it can be modified for the summation of series with alternating signs, for the evaluation of limits and derivatives and for extrapolation when the expansion has general term $a_j h^{j\gamma+\delta}$ (see § 15 (above)). Then he showed how to derive multipliers for obtaining individual elements in extrapolation schemes without computing the others and concluded by investigating the behavior of truncation error and rounding error, discussing the optimal choice of arguments.

18. Algorithms. BAUER (1961a,b) appears to have been the first to publish an algorithm for Romberg quadrature. His ALGOL procedure carried out the usual Romberg process, with $r_k = 2^{-k}$, to a specified order. DUNKL (1963) wrote a FORTRAN routine which incorporated a relative error test (as suggested by THACHER (1962a)) and required the specification of a minimum, as well as a maximum, order. LAURENT (1963c, 1964b) gave an ALGOL procedure for numerical integration in two dimensions. BULIRSCH (1964) used $\{r_k\} = Q$ for quadrature to a specified order, and GRAM (1964) corrected for rounding error, using $r_k = 2^{-k}$ and a relative error test.

BULIRSCH and STOER (1964) used rational extrapolation with $\{r_k\} = Q$ and ELLIOT and PRAGER (1965) implemented the adaptive routine described in § 15 (above). KUBIK (1965) used polynomial extrapolation with $r_k = 2^{-k}$, testing $|T_m^0 - U_m^0|$ and stopping when it was small enough, and BULIRSCH and STOER (1967b) included a similar convergence criterion in an algorithm based on rational extrapolation with $\{r_k\} = Q$. HAVIE (1967) modified Kubik's algorithm to allow the use of the cosine transformation (see § 15 (above)), and HILLSTROM (1968a) wrote a FORTRAN subroutine which offered a choice of four convergence tests.

FAIRWEATHER (1969) made use of two devices designed to reduce rounding error: the "skeleton table" suggested by KRASUN and PRAGER (1965) (see § 15 (above)), and the procedure for evaluating the U_0^i introduced by RUTISHAUSER (1967). WALLICK (1970a,b) found experimentally that the latter has greater effect. Other programs have been published by CONTE (1965), WELSCH (1966), CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE (1967), MCCALLA (1967), WILF (1967), CARNAHAN, LUTHER and WILKES (1969) and WANG (1969).

Tests and comparisons with other quadrature methods have been reported by KAPFER (1966), HILLSTROM (1966, 1967, 1968b), FARKAS (1966), TOMPA (1967, 1969), HOPEWELL (1967), MIKLOSKO (1967), BABUSKA (1968a,b), CODY and HILLSTROM (1968), O'HARA and SMITH (1968, 1969), LYNESS (1968a, 1969a,b,c), SMITH and LYNESS (1969), ROBINSON (1969), KAHANER (1969), AMBLE (1969), BRAKHAGE and BROMBEER (1969), CASALETTO, PICKETT and RICE (1969), HAVIE (1969b), MILLER (1970), COOK (1970), and OLIVER (1971).

Published algorithms for the numerical solution of IV problems in ODE's include those of LAURENT (1964b), MCCALLA (1967) and ASWANI (1967), which use Euler's method, and that of BULIRSCH and STOER (1966a), which uses the Gragg–Stoer method with automatic step-size correction and $\{r_k\} = Q$ (see § 14 (above)). This last algorithm has been adapted for use as a FORTRAN function by CLARK (1968) and CRANE and FOX (1969a,b). SMITH and MCCALL (1970) applied extrapolation to Massau's method for hyperbolic PDE's.

LAURENT (1964b) also gave ALGOL procedures for numerical differentiation using polynomial extrapolation, and for extrapolation by the methods of Lagrange, Neville and Newton (see § 5 (above)). STAFFORD (1965) and BOOTHROYD (1966) published interpolation algorithms based on the processes of Aitken and Neville. WINRICH (1969) and KROGH (1970) compared the efficiency of several schemes for interpolation including Aitken's and Neville's.

19. Concluding remarks. As was pointed out at the beginning, this survey is concerned mainly with extrapolation processes based on polynomial or rational

functions. In the interests of brevity, not all cited papers have been discussed in detail and there are, no doubt, some gaps in the bibliography. The reader interested in other convergence acceleration techniques, such as the ε-algorithm, will find useful bibliographies in the papers of WYNN (1956c, 1963) and GRAY and CLARK (1969).

It is noticeable that there has been a certain amount of rediscovery and it is unfortunate that the papers of SHEPPARD (1900), AITKEN (1932b, 1938), NEVILLE (1934) and ROMBERG (1955) have not had wider circulation. Romberg, in particular, covered rather more ground than is generally believed, investigating sequences other than $\{r_k = 2^{-k}\}$, and pointing out the usefulness of the U_m^i, both for efficient computation and for error estimation.

Perhaps the three most useful developments of the last 15 years are:

(a) the modification of Romberg's method to deal with integrals with singularities (see § 10 (above));

(b) the modification of the midpoint method to allow the use of $(h^2, h^4, \cdots)$-extrapolation in the solution of IV problems in ODE's (see § 14 (above)); and

(c) the exploitation of asymptotic upper and lower bounds (see § 16 (above)).

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