

Integration over multidimensional hypercubes

I. A progressive procedure

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A method of numerical integration is described which uses a low order integration rule to obtain a high order result. The error is successively reduced, using a method based on the idea of Richardson's deferred approach to the limit. The method is restricted to hypercubic domains.

The standard methods of multidimensional numerical integration require the evaluation of the function at a number of points. The effort spent is normally directly proportional to the number of such evaluations, and consequently it is desirable to obtain an accurate result with as few function evaluations as possible.

Methods based on random procedures, such as the Monte Carlo method (Davis and Rabinowitz, 1956), and the recent method using Cesaro Sums (Haselgrove, 1961,) are easy to code and, as the number of points is increased, convergence of successive results may be observed directly. Such methods permit the use of additional points to increase the accuracy of a result and provide a convenient statistical estimate of the error.

Systematic methods based on integration rules do not usually have these advantages and, in fact, very few high order (order > 5) multidimensional rules are known (Hammer and Stroud, 1958). It is usual to use a low order rule over a fine mesh and often the mesh size is arbitrarily chosen. The error estimates of these methods are in a form which is difficult to use.

In this paper, we outline a simple progressive procedure for integration over hypercubic domains by which any systematic low order integration rule may be used to yield a high order result. This method consists of a process of elimination of errors, based on the idea of the deferred approach to the limit of Richardson. In Section 1, we describe the method in detail in one dimension and illustrate it with a simple example. In Section 2, we give a general description of the method and, in Section 3, we apply it to a five-dimensional numerical example.

1. The progressive procedure in one dimension

The method which we describe in general in Section 2 is a useful and powerful tool for carrying out numerical integration in many dimensions. In the interests of clarity, we devote this section to describing the method in one dimension and illustrating its use by means of a simple example. This description is primarily intended to clarify the technique. The value of the method is more apparent in many dimensions, where its efficiency compares favourably with other procedures.

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We suppose that we wish to evaluate numerically the integral

$$I = \int_0^1 f(x) dx. \quad (1.1)$$

A simple approach is to divide the interval (0,1) into r equal intervals of length $1/r$ and to use a mid-point rule for each interval. Thus we write

$$\int_{i/r}^{(i+1)/r} f(x) dx \doteq \frac{1}{r} f\left(\frac{2i+1}{2r}\right) \quad (1.2)$$

for each interval and, combining these results, we obtain an approximation $I(r)$ to the true integral I . This we may express as

$$I \doteq I(r) = \frac{1}{r} \left\{ f\left(\frac{1}{2r}\right) + f\left(\frac{3}{2r}\right) + \dots + f\left(\frac{2r-1}{2r}\right) \right\}. \quad (1.3)$$

In general, this is rather an inefficient method for carrying out an integration. The first few approximations to

$$I = \int_0^1 \exp(-3x) dx$$

obtained using this method are listed in Table 1. There it is seen that, using ten function evaluations, the numerical result differs from the exact result by about one part in three hundred.

Table 1

The approximation $I(r)$ given by (1.3) to I given by (1.1) when $f(x) = \exp(-3x)$

| r | $I(r)$ | NUMBER OF POINTS |
|----------------|----------|------------------|
| 1 | 0.223130 | 1 |
| 2 | 0.288883 | 2 |
| 3 | 0.303915 | 3 |
| 4 | 0.309434 | 4 |
| 10 | 0.315553 | 10 |
| $I = 0.316738$ | | |

We may obtain closer numerical results if we calculate the same approximations $I(r)$, but combine them in an advantageous way, that is in the same way as is used in integrating differential equations, using Richardson's deferred approach to the limit. An elementary application of the Euler-Maclaurin expansion to each interval in turn leads to the result

$$I(r) = I + \frac{\beta_2}{r^2} + \frac{\beta_4}{r^4} + \frac{\beta_6}{r^6} + \dots \quad (1.4)$$

Expressions for β_{2s} are given in Milne Thomson (1933). β_{2s} depends on $f(x)$ and on the rule (in this case (1.2)), but is independent of r . In order to simplify the discussion, we assume for the moment that expansion (1.4) converges for integer r , though this assumption is not necessary. We may write $r = 1$ and $r = 2$ in (1.4) to obtain

$$J_1 = I(1) = I + \beta_2 + \beta_4 + \beta_6 + \dots \quad (1.5)$$

$$I(2) = I + \frac{1}{4}\beta_2 + \frac{1}{16}\beta_4 + \frac{1}{64}\beta_6 + \dots \quad (1.6)$$

These equations may be combined to eliminate β_2 , yielding

$$J_2 = -\frac{1}{3}I(1) + \frac{4}{3}I(2) = I - \frac{1}{4}\beta_4 - \frac{5}{16}\beta_6 - \dots \quad (1.7)$$

To carry the procedure one stage further, we substitute $r = 3$ in (1.4) to obtain

$$I(3) = I + \frac{1}{9}\beta_2 + \frac{1}{81}\beta_4 + \frac{1}{729}\beta_6 + \dots \quad (1.8)$$

and combine (1.5), (1.6) and (1.8) in such a way that we eliminate β_2 and β_4 . The result is

$$J_3 = \frac{1}{24}I(1) - \frac{16}{15}I(2) + \frac{81}{40}I(3) = I + \frac{1}{36}\beta_6 + \dots \quad (1.9)$$

The procedure described above to generate J_1 , J_2 and J_3 is a progressive procedure. In general, if we have calculated $I(r)$ $r = 1, 2 \dots p$, we may determine numbers γ_{pr} so that

$$J_p = \sum_{r=1}^p \gamma_{pr} I(r) = I + E_{pp}\beta_{2p} + E_{pp+1}\beta_{2p+2} + \dots \quad (1.10)$$

The coefficients γ_{pr} and expressions for E_{ps} are listed in the Appendix (A.16, A.12 and Table 5).

In Table 2, we list the first four values of J_p obtained from the corresponding values of $I(r)$ in Table 1.

It should be expected that J_r is closer than $I(r)$ to I as, in general, more function evaluations are required to determine J_r . However, comparison of Tables 1 and 2 shows that, from the point of view of efficiency, the progressive procedure is very much better. For example, J_4 differs from I by less than one part in 100,000, compared with the one part in 300 by which

Table 2

The approximations J_p given by (1.10) to I given by (1.1) when $f(x) = \exp(-3x)$

| p | J_p | NUMBER OF POINTS |
|----------------|----------|------------------|
| 1 | 0.223130 | 1 |
| 2 | 0.310801 | 3 |
| 3 | 0.316584 | 5 |
| 4 | 0.316736 | 9 |
| $I = 0.316738$ | | |

$I(10)$ differs from I . But J_4 in fact requires fewer function evaluations than $I(10)$.

The reason for this improvement is easily explained. We may define a rule for which $\beta_2 = \beta_4 = \dots = \beta_{2t} = 0$ as a rule "of order $2t + 1$ ". Such a rule integrates exactly all polynomials of degree $2t + 1$. In this case, the rule we are using (1.2) is a first order rule. However, (1.7) and (1.9) indicate that J_2 and J_3 correspond to third and fifth order rules respectively. Thus, if $f(x)$ were a polynomial of degree 5, J_3 would be exactly equal to I , while any of $I(1)$, $I(2)$ or $I(3)$ would differ from I .

The procedure described above is powerful and practical. It makes full use of all previous function evaluations and provides a visual check on the convergence. The normal integration procedures have disadvantages when put into practice. For example the integrator does not know in advance what interval to use or what order rule to use. He usually determines this by trial and error with the result that, although the final rule he need use may be marginally more efficient than the progressive procedure, he has, in fact, carried out many more function evaluations than he needed by searching for this most efficient rule and establishing that it is accurate enough.

The principal drawback of the progressive procedure lies in the build-up of rounding errors, due to the difference in magnitudes of γ_{pr} . Reference to the tabulated values of γ_{pr} in the Appendix (Table 5) indicates that, if $I(r)$ is evaluated to n decimal places, J_6 is accurate to $(n - 1)$ places and J_9 to $(n - 2)$ places. Thus care must be taken to carry sufficient figures. This presents no difficulty for an electronic computer, but may be very inconvenient for a hand computation.

The question of rounding errors using this progressive procedure will be treated in greater detail in a forthcoming publication.

There is no need to use rule (1.2) in each interval. We may replace (1.2) by any other rule of order one or more that we like to invent. If we use a first order rule the procedure is identical to that described above and the results are of the various orders stated above. If we use a higher order rule, again the above procedure may be

used, but unless modified, it is not the most efficient. For example, Simpson's three-point third order rule applied to each interval leads to

$$I(r) = \frac{1}{6r} \left\{ f(0) + 4f\left(\frac{1}{2r}\right) + 2f\left(\frac{2}{2r}\right) + 4f\left(\frac{3}{2r}\right) + \dots + 4f\left(\frac{2r-1}{2r}\right) + f(1) \right\}. \quad (1.11)$$

The Euler-Maclaurin expansion analogous to (1.2) is

$$I(r) = I + \frac{\beta_4}{r^4} + \frac{\beta_6}{r^6} + \dots$$

The β_2 term is zero, as Simpson's rule is a third order rule.

If we were to carry out an identical procedure to that above we would eliminate the non-existent term β_2 to obtain a third order result from two results already of third order. It is clearly more advantageous to make use of the knowledge that $\beta_2 = 0$ and to eliminate the β_4 term instead. Thus the procedure is the same, but the coefficients $\gamma_{pr}^{(1)}$ replace γ_{pr} . The resulting equations, analogous to (1.7) to (1.9) above are

$$I(1) = I + \beta_4 + \beta_6 + \dots$$

$$I(2) = I + \frac{1}{16}\beta_4 + \frac{1}{64}\beta_6 + \dots$$

combining these we find

$$J_2 = -\frac{1}{15}I(1) + \frac{16}{15}I(2) = I - \frac{1}{20}\beta_6 - \dots$$

In general

$$J_p = \sum_{r=1}^p \gamma_{pr}^{(1)} I(r) = I + \sum_{s=p+1} E_{ps}^{(1)} \beta_{2s}$$

and here J_p is a $(2p+1)$ th order result.

In general, if the rule to be used is of order $(2t+1)$, the procedure should be modified by replacing γ_{pr} by $\gamma_{pr}^{(t)}$, and the p th result J_p is a result of order $(2p+2t-1)$.

The results using Simpson's rule corresponding to those in Tables 1 and 2 are given in Table 3. In this case, it is seen that, from the point of view of efficiency, there is little to choose between using the third order or first order rule, if used in this way for this particular example. The question of which rule is preferable in practice will be discussed in a forthcoming publication.

Finally, we should draw attention to an additional flexibility of the method. If the function to be integrated is tabulated, it may be possible to choose integration intervals which restrict the required function evaluation to points at which the function is tabulated. To arrange this would require a progression which might differ from $r=1, 2, 3, \dots$. The necessary coefficients $\gamma_{pr}^{(t)}$ for any progression are given by formulae (A. 11) and (A. 14) of the Appendix.

Table 3

The numerical results corresponding to Tables 1 and 2 when the third order rule (1.11) is used

| DIRECT | | | COMBINED | |
|----------------|----------|------------------|--------------|------------------|
| $r = p$ | $I(r)$ | NUMBER OF POINTS | J_p | NUMBER OF POINTS |
| 1 | 0.323718 | 3 | 0.323718 | 3 |
| 2 | 0.317259 | 5 | 0.316828 | 5 |
| 3 | 0.316844 | 7 | 0.316738 | 9 |
| $I = 0.316738$ | | | $= 0.316738$ | |

2. The progressive procedure in n dimensions

To obtain an approximation to the integral of the function $f(\vec{x}) = f(x_1, x_2, \dots, x_n)$ over an n -dimensional hypercubic domain D of side $2a$ ($|x_i| < a; i = 1, 2, \dots, n$), we first divide the domain into $N = r^n = (a/h)^n$ equal hypercubic subdomains S_i of side $2h$ and centre \vec{c}_i . (We term r the mesh ratio and h the mesh size.) We then evaluate the integral by applying an integration rule (Miller, 1960; Mustard, Lyness and Blatt, 1963) over each subdomain and calculate

$$(2h)^n \sum_{j=1}^m w_j f(\vec{c}_i + h\vec{\alpha}_j) \doteq \int_{S_i} f(\vec{x}) dx_1, dx_2, \dots, dx_n$$

where the m weights w_j and vectors $\vec{\alpha}_j$ are given by the rule. Summing over the N subdomains gives an approximation $I(r)$ to the exact integral I as follows:

$$I = \int_D f(\vec{x}) dx_1, dx_2, \dots, dx_n \doteq I(r) = (2h)^n \sum_{i=1}^N \sum_{j=1}^m w_j f(\vec{c}_i + h\vec{\alpha}_j). \quad (2.1)$$

We assume in this paper that the function $f(\vec{x})$ is one for which all partial derivatives of order $2q$ or less are continuous within the domain D . (This condition is probably over-restrictive.) The difference $I(r) - I$ may then be expanded in a finite power series in even inverse powers of the mesh ratio r , with a remainder of order r^{-2q} . For a symmetrical rule of order $2t+1$, this expansion takes the form

$$I(r) = I + \sum_{s=t+1}^{q-1} \beta_{2s} r^{2s} + R_{2q}(r) \quad (2.2)$$

where

$$\beta_{2s} = a^{2s} \sum_{\Sigma s_i = s} c_{2s_1, 2s_2, \dots, 2s_n} \times \int_D \frac{\partial^{2s} f}{\partial x_1^{2s_1} \partial x_2^{2s_2} \dots \partial x_n^{2s_n}} dx_1 dx_2 \dots dx_n.$$

Thus β_{2s} depends linearly on the integrals over the domain of partial derivatives of order $2s$, the coefficients

depending on the particular rule. Expressions for these coefficients are given in a forthcoming paper; there it is shown that $R_{2q}(r)$ may be expressed in terms of weighted integrals over the domain of partial derivatives of order $2q$, so long as $2q > n$. It is easy to verify that, if the rule used is of order $2t + 1$, all of the coefficients $c_{2s_1, 2s_2, \dots}$ for which $\sum s_i < t$ are zero, with the result

$$\beta_{2s} = 0 \quad s < t.$$

As the coefficients β_{2s} in (2.2) are independent of r , the mesh ratio, we may proceed as follows. We may compute two separate values $I(r_1)$ and $I(r_2)$ using distinct mesh ratios r_1 and r_2 . Both of these are approximations to I and each satisfies equation (2.2). We may then eliminate the first non-zero error term β_{2t+2} from these equations. This gives us a value J_2 which satisfies equation (2.5) below and which forms the first step in the process.

At the p th stage of this process, we have already carried out $p - 1$ distinct numerical integrations with distinct mesh ratios r_1, r_2, \dots, r_{p-1} giving results $I(r_i)$ of the form (2.1). The p th step is to choose another distinct mesh ratio r_p to calculate $I(r_p)$ and combine this result with the previous $(p - 1)$ results to eliminate $\beta_{2s}(s = t + 1, \dots, t + p - 1)$. Thus we have the p th value J_p given by

$$J_p = \sum_{i=1}^p \gamma_{pi}^{(i)} I(r_i) \quad (2.3)$$

where

$$\sum_{i=1}^p \gamma_{pi}^{(i)} = 1 \quad (2.4)$$

and

$$\sum_{i=1}^p \gamma_{pi}^{(i)} r_i^{-2s} = 0 \quad s = t + 1, t + 2, \dots, t + p - 1.$$

The coefficients $\gamma_{pi}^{(i)}$ are defined by (2.4). They are independent of the integral to be evaluated and of n , the number of dimensions (which occurs in the definition of β_{2s}); they are algebraic functions of the mesh ratios r_1, r_2, \dots, r_p . Expressions for $\gamma_{pi}^{(i)}$ are given in the Appendix.

The process may be continued until successive values J_{p-1} and J_p differ by less than the required tolerance.

The expansion for J_p in terms of β_{2s} is

$$J_p = I + \sum_{s=t+p}^{q-1} \beta_{2s} \left(\sum_{i=1}^p \gamma_{pi}^{(i)} r_i^{-2s} \right) + \sum_{i=1}^p \gamma_{pi}^{(i)} R_{2q}(r_i). \quad (2.5)$$

We see that $J_p - I$ is independent of derivatives of $f(x)$ of order $2t + 2p - 1$ or less. Thus, in view of (2.2), J_p is a $(2t + 2p - 1)$ th order result. It is, in fact, the result which would have been obtained using a complicated high order rule. This high order rule assigns weights $w_j \gamma_{pi}^{(i)} / r_i^{2j}$ to each of the mr_i^n points required by the low order rule (2.1) when the mesh ratio is r_i . In this sense, we may consider this process as a generator of high order integration rules.

To minimize the number of function evaluations we make our mesh ratios as small as possible by choosing

Table 4

Approximations $I(r)$ and J_r to

$$I = \int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 \exp(-x_1 x_2 x_3 x_4 x_5) dx_1 dx_2 dx_3 dx_4 dx_5.$$

The expression for $I(r)$ is

$$I(r) = \frac{1}{r^5} \sum_{i=1}^r \sum_{j=1}^r \sum_{k=1}^r \sum_{l=1}^r \sum_{m=1}^r \exp \left[-\frac{2i-1}{2r} \cdot \frac{2j-1}{2r} \cdot \frac{2k-1}{2r} \cdot \frac{2l-1}{2r} \cdot \frac{2m-1}{2r} \right]$$

and the values of J_r are obtained from (2.3) using the values of γ_{pr} listed in Table 5.

| DIRECT | | | COMBINED | |
|-------------------|-------------|------------------|-----------------|-------------------|
| r | $I(r)$ | NUMBER OF POINTS | J_r | NUMBER OF POINTS* |
| 1 | 0.969233234 | 1 | 0.969233234 | 1 |
| 2 | 0.970160833 | 32 | 0.970470032 | 33 |
| 3 | 0.970422763 | 243 | 0.970652591 | 276 |
| 4 | 0.970522498 | 1024 | 0.970657153 | 1300 |
| 5 | 0.970570137 | 3125 | 0.970657188 | 4425 |
| $I = 0.970657191$ | | | $= 0.970657191$ | |

the progression $r_i = i$. Investigations of other progressions are incomplete, but tend to indicate that, while greater accuracy may be obtained, this is at the expense of an increase in the number of function evaluations. The optimum progression and the related question of the choice of integration rule are discussed in a forthcoming publication.

3. A numerical example in 5 dimensions

To illustrate the procedure, we chose the same example as that used by Haselgrove (1961), namely the five-dimensional integral

$$\int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 \exp(-x_1 x_2 x_3 x_4 x_5) dx_1 dx_2 dx_3 dx_4 dx_5 \quad (3.1)$$

and evaluated it using the simplest first order rule, the centre rule, and the mesh ratio progression $r_i = i$.

The necessary calculations were carried out on the UTECOM (Deuce) computer of the University of New South Wales. The function was calculated to nine decimals and the summation was carried out using double-length addition to reduce the accumulation of round-off errors. In calculating the combined results by (2.3), nine decimal figures were retained. A suitable constant was subtracted from the $I(r)$ before combination. This procedure was found to give results reliable to at least eight decimal places.

The values of $I(r)$ and J_r for $r = 1 \dots 5$ are given in

* The small number of points common to certain meshes has not been deducted.

Table 4 with the corresponding numbers of function evaluations.

The values of J_r and the number of points at which function evaluation was necessary may be compared with Table 3, p. 336 of Haselgrove (1961). There it is found that the unmodified Monte Carlo method gives a result accurate to four decimal places after 12,000 points. Haselgrove obtains results accurate to four decimal places using 4,000 points, and six decimal places using 12,000 points. The convergence of J_r in Table 4 above is faster than this, yielding six decimal places in 1,300 points, and eight decimal places after 4,425 points.

The integrand in (3.1) is a smooth well-behaved function. In general this may not be the case. The efficiency of this progressive procedure is strongly dependent on the behaviour of the function and its derivatives.

If the function itself contains a singularity, this method is not valid unless the form of the singularity is known and it is in some way "factored out".

A near singularity is characterized by large derivatives and large values of β_{2p} ; in this case the progression J_2, J_3, \dots should converge only in an unsystematic manner, and this should indicate how far the results may be taken seriously. It is still possible to be seriously misled. An example is the integrand

$$f(\vec{x}) = g(\vec{x}) + h(\vec{x}) \cos \{60 \pi x_1\}$$

with the domain of integration $|x_i| < 1$.

The centre rule would evaluate this function at points where $\cos 60 \pi x_1$ is unity for mesh ratios $r = 1, 2, 3, 4, 5$ and 6. Thus the values of J would approach the integral of $g(\vec{x}) + h(\vec{x})$ until we chose a higher mesh ratio. In this case the existence of a regular pattern of what may be termed equal and opposite near singularities leads to deceptive indications about the value of the numerical results.

Finally, if the function has any discontinuous derivatives of order $2p'$ or $2p' - 1$, this progressive procedure ceases to be powerful when the number of steps p exceeds p' . This is because the term β_{2p} contains the integral of these derivatives and so $\beta_{2p'+2}$ does not exist. Thus we are eliminating non-existent terms to obtain $J_{p'+1}$ and there is no reason to suppose that $J_{p'+1}$ is a very marked improvement of J_p . However, since the progressive procedure may be regarded as the generator of an integration rule, the procedure does not break down. In general a result based on a larger number of function evaluations is likely to be better. The effect of non-continuous derivatives is to alter the rate of convergence, which should be fast until $J_{p'}$ is reached and slow thereafter.

In spite of the possibility of being misled, we recommend the use of this progressive procedure until it appears to have converged. Detailed expressions for both an error bound and an error estimate will be presented in a forthcoming publication. However, these expressions are of little practical utility, except when used to compare different integration procedures.

Table 5

The numerical values of γ_{ps} for a first-order integration rule and mesh ratio progression $i = 1, 2, \dots, p$.

| p | s | NUMERATOR/DENOMINATOR | VALUE |
|-----|-----|---------------------------|-----------------------|
| 1 | 1 | + 1 | + 1. 00000 00000 00 |
| | D | 1 | |
| 2 | 1 | - 1 | - 0. 33333 33333 33 |
| | 2 | + 4 | + 1. 33333 33333 33 |
| | D | 3 | |
| 3 | 1 | + 5 | + 0. 04166 66666 67 |
| | 2 | - 128 | - 1. 06666 66666 67 |
| | 3 | + 243 | + 2. 02500 00000 00 |
| | D | 120 | |
| 4 | 1 | - 7 | - 0. 00277 77777 78 |
| | 2 | + 896 | + 0. 35555 55555 56* |
| | 3 | - 6561 | - 2. 60357 14285 71 |
| | 4 | + 8192 | + 3. 25079 36507 94 |
| | D | 2520 | |
| 5 | 1 | + 42 | + 0. 00011 57407 41 |
| | 2 | - 24576 | - 0. 06772 48677 25 |
| | 3 | + 5 31441 | + 1. 46450 89285 71 |
| | 4 | - 20 97152 | - 5. 77918 87125 22 |
| | 5 | + 19 53125 | + 5. 38228 89109 35 |
| | D | 3 62880 | |
| 6 | 1 | - 66 | - 0. 00000 33068 78 |
| | 2 | + 1 68960 | + 0. 00846 56084 66* |
| | 3 | - 97 43085 | - 0. 48816 96428 57 |
| | 4 | + 922 74688 | + 4. 62335 09700 18 |
| | 5 | - 2441 40625 | - 12. 23247 47975 79 |
| | 6 | + 1813 98528 | + 9. 08883 11688 31 |
| | D | 199 58400 | |
| 7 | 1 | + 429 | + 0. 00000 00688 93 |
| | 2 | - 46 85824 | - 0. 00075 24985 30 |
| | 3 | + 6839 64567 | + 0. 10983 81696 43 |
| | 4 | - 1 39586 43712 | - 2. 24162 47127 36 |
| | 5 | + 7 93457 03125 | + 12. 74216 12474 78 |
| | 6 | - 15 67283 28192 | - 25. 16907 09290 71 |
| | 7 | + 9 68890 10407 | + 15. 55944 86543 23 |
| | D | 62270 20800 | |
| 8 | 1 | - 715 | - 0. 00000 00010 94 |
| | 2 | + 328 00768 | + 0. 00005 01665 69 |
| | 3 | - 1 17517 54833 | - 0. 01797 35186 69 |
| | 4 | + 48 85525 29920 | + 0. 74720 82375 79 |
| | 5 | - 534 05761 71875 | - 8. 16805 20817 17 |
| | 6 | + 2115 83243 05920 | + 32. 36023 40516 63 |
| | 7 | - 3323 29305 69601 | - 50. 82753 22707 88 |
| | 8 | + 1759 21860 44416 | + 26. 90606 54164 57 |
| | D | 65 38371 84000 | |
| 9 | 1 | + 4862 | + 0. 00000 00000 14 |
| | 2 | - 9269 41184 | - 0. 00000 26060 56 |
| | 3 | + 79 91193 28644 | + 0. 00224 66898 34 |
| | 4 | - 6542 09418 52672 | - 0. 18392 81815 58 |
| | 5 | + 1 29699 70703 12500 | + 3. 64645 18221 95 |
| | 6 | - 9 20810 27379 36384 | - 25. 88818 72413 30 |
| | 7 | + 27 68303 11644 77633 | + 77. 82965 87896 44 |
| | 8 | - 36 02879 70189 63968 | - 101. 29342 27443 09 |
| | 9 | + 16 67718 16996 66569 | + 46. 88718 34715 66 |
| | D | 35568 74280 96000 | |
| 10 | 1 | - 8398 | - 0. 00000 00000 00 |
| | 2 | + 66044 55936 | + 0. 00000 01085 86 |
| | 3 | - 1351 47763 38276 | - 0. 00022 22000 93 |
| | 4 | + 2 13085 35346 29888 | + 0. 03503 39393 44 |
| | 5 | - 73 92883 30078 12500 | - 1. 21548 39407 32 |
| | 6 | + 885 70438 21052 55936 | + 14. 56210 53232 48 |
| | 7 | - 4548 15917 89638 84057 | - 74. 77751 53076 97 |
| | 8 | + 10952 75429 37650 46272 | + 180. 07719 59898 82 |
| | 9 | - 12157 66545 90569 28801 | - 199. 88746 63787 81 |
| | 10 | + 5000 00000 00000 00000 | + 82. 20635 24662 43 |
| | D | 60 82255 02044 16000 | |

γ_{ps} may be expressed as a fraction N_{ps}/D_p ; the values of N and D are given, together with the decimal value rounded to twelve places of decimals.

* This number should be reduced by 1 in the final decimal places if it is required to arrange γ_{ps} so that

$$\sum_{s=1}^p \gamma_{ps} = 1.00000 00000 00$$

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Appendix

The coefficients $\gamma_{pi}^{(t)}$

The coefficients $\gamma_{pi}^{(t)}$ defined by (2.4) are algebraic functions of the p distinct mesh ratios r_1, r_2, \dots, r_p . For convenience, we substitute

$$x_i = 1/r_i^2 \quad (\text{A.1})$$

and equation (2.4) may be written

$$\sum_{i=1}^p \gamma_{pi}^{(t)} = 1$$

$$\sum_{i=1}^p \gamma_{pi}^{(t)} x_i^s = 0 \quad s = t+1, \dots, p+t-1 \quad (\text{A.2})$$

and we define the coefficient occurring in expansion (2.5)

$$\sum_{i=1}^p \gamma_{pi}^{(t)} x_i^s = E_{ps}^{(t)} \quad s = p+t, p+t+1, \dots \quad (\text{A.3})$$

The equations (A.2) are usually unsuitable for accurate calculation of $\gamma_{pi}^{(t)}$ by direct numerical solution of the p linear equations, as these equations are likely to be ill-conditioned. We list here expressions suitable for their numerical evaluation. We do not give the derivation in detail, but we indicate the method by listing the algebraic results used. These results are derived in Milne-Thompson (1933), and are as follows.

A partial-fraction theorem states that, if x_1, x_2, \dots, x_d are distinct and $g(x)$ is a polynomial of positive degree $d-2$ or less, then

$$\sum_{r=1}^d \frac{g(x_r)}{\prod_{i \neq r} (x_i - x_r)} = 0. \quad (\text{A.4})$$

The extension of the Van der Monde determinant

$$\begin{vmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \\ \vdots & \vdots & \dots & \vdots \\ x_1^{n-2} & x_2^{n-2} & \dots & x_n^{n-2} \\ x_1^{n-1+s} & x_2^{n-1+s} & \dots & x_n^{n-1+s} \end{vmatrix} = D_s^n(x_1, x_2, \dots, x_n) \quad (\text{A.5})$$

where x_1, x_2, \dots, x_n are distinct and s is a non-negative integer has the following factorization:

$$D_s^n(x_1, x_2, \dots, x_n) = D_0^n(x_1, x_2, \dots, x_n) F_s^n(x_1, x_2, \dots, x_n) \quad (\text{A.6})$$

where

$$D_0^n(x_1, x_2, \dots, x_n) = \prod_{j>i}^n (x_j - x_i). \quad (\text{A.7})$$

$F_s^n(x_1, x_2, \dots, x_n)$ is the sum of the homogeneous products of order s of x_1, x_2, \dots, x_n . Thus

$$F_s^n(x_1, x_2, \dots, x_n) = \sum x_1^{s_1} x_2^{s_2} \dots x_n^{s_n} \quad (\text{A.8})$$

where the summation is extended to all positive integers, including zero, which satisfy the relation

$$s_1 + s_2 + \dots + s_n = s. \quad (\text{A.9})$$

In the notation of Milne-Thompson, $F_s^n(x_1, x_2, \dots, x_n)$ is the divided difference $[x_1 x_2 \dots x_n]$ of the function x^s . This function has the expansion

$$F_s^n(x_1, x_2, \dots, x_n) = (-1)^{n-1} \sum_{r=1}^n \frac{x_r^{n+s-1}}{\prod_{i \neq r} (x_i - x_r)}. \quad (\text{A.10})$$

Using these relationships, we may obtain expressions for the first order coefficients; these are

$$\gamma_{pr}^{(0)} = \left\{ \prod_{i \neq r} \left(1 - \frac{x_r}{x_i} \right) \right\}^{-1} \quad (\text{A.11})$$

$$E_{ps+p}^{(0)} = (-1)^{p-1} \prod_{i=1}^p x_i F_p^{(0)}(x_1, x_2, \dots, x_p) \quad (\text{A.12})$$

and we find that $(-1)^{p-1} E_{ps}^{(0)}$ is bounded and monotonic increasing in s , bounded by

$$(-1)^{p-1} E_{pp}^{(0)} x_1^p < (-1)^{p-1} E_{ps}^{(0)} < (-1)^{p-1} \gamma_{p1}^{(0)} x_1^{p+p} \quad (\text{A.13})$$

where x_1 is the maximum of the positive numbers x_1, x_2, \dots, x_p .

The corresponding quantities for higher order coefficients ($t > 0$) are given in terms of those for $t = 0$ by

$$\gamma_{pr}^{(t)} = \gamma_{pr}^{(0)} \left\{ x_r^t F_p^{(0)} \left(\frac{1}{x_1}, \frac{1}{x_2}, \dots, \frac{1}{x_p} \right) \right\}^{-1} \quad (\text{A.14})$$

$$E_{ps+t}^{(t)} = E_{ps}^{(0)} \left\{ F_p^{(0)} \left(\frac{1}{x_1}, \frac{1}{x_2}, \dots, \frac{1}{x_p} \right) \right\}^{-1}. \quad (\text{A.15})$$

The values of $\gamma_{ps}^{(0)}$ for the sequence

$$x_i = 1/i^2 \quad i = 1, 2, \dots, p$$

that is, for the mesh ratio sequence $r_i = i$ are

$$\gamma_{ps} = \frac{2s^{2p} (-1)^{p-s}}{(p+s)! (p-s)!} = (-1)^{p-s} \frac{2s^{2p}}{(2p)!} \binom{2p}{s+p}. \quad (\text{A.16})$$

These coefficients are of widely different magnitudes. The largest value of $|\gamma_{ps}|$ for a fixed p occurs near $s = s_0$, where

$$s_0 = \frac{1}{2} + \left[\frac{1}{4} + \frac{2p^2(p+1)}{4p+1} \right]^{\frac{1}{2}} \approx \frac{p}{\sqrt{2}}. \quad (\text{A.17})$$

We introduce coefficients $L_p^{(i)}$ useful for discussing the convergence of the iteration process. We may write

$$L_p^{(0)} = \sum_{s=1}^p \frac{|\gamma_{ps}^{(0)}|}{s^{2p}} = \frac{2^{2p}}{(2p)!} N_p \quad (\text{A.18})$$

where

$$N_p = 1 - \frac{(2p-1)!!}{(2p)!!} \approx 1. \quad (\text{A.19})$$

The values of $\gamma_{ps}^{(i)}$ for this mesh ratio sequence may be easily obtained using (A.14), and the value of $L_p^{(i)}$ is given by

$$L_p^{(i)} = \sum_{s=1}^p \frac{|\gamma_{ps}^{(i)}|}{s^{2(p+i)}} = L_p^{(0)} \{F_p^{(i)}(1, 4, 9, \dots, p^2)\}^{-1}. \quad (\text{A.20})$$

We should like to acknowledge helpful discussions with Professor J. M. Blatt and Dr. L. M. Delves.

Book Reviews (continued from p. 263)

state of progress in U.K. as compared with U.S.A., and it is perhaps sad that, since in the preface to Vol. 2 the editor wrote that Vol. 1 reflects the backward state of automatic programming methods in U.K., we do not seem to have progressed very much further forward.

The paper on RAPIDWRITE describes a worthwhile effort, although it does not present any new information, and most of those who are interested may wish to seek elsewhere for their description. The language SEAL comes back for a follow-up from Vol. 2 but one still feels that it is somewhat out in the cold. The problem which yet remains to be solved is to what extent commercial users dare depart from COBOL, and also to what extent a language unique to one machine can be allowed to propagate a growth of programs which are not interchangeable.

This volume has maintained the standard of its predecessor, also with an increase in price, but the timing of the next volume and the selection of papers still merit all the editor's skill if the publication is to remain fresh. B. RICHARDS

Proceedings of a Harvard Symposium on Digital Computers and Their Applications. Edited by A. G. OETTINGER, 1962; 332 pages. (London: Oxford University Press, 120s. Cambridge, Mass. Harvard University Press)

The Proceedings of the first two Harvard Symposia on digital computers occupy respected places in the libraries of computing laboratories, and this volume, the Proceedings of a Symposium held in April, 1961, may be expected to gain similar acceptance. This Symposium was, however, quite different from the others. Previously the design and hardware aspects of computers had occupied substantial time and so, too, had reports of problems in Numerical Analysis and applications to the physical sciences. This time much greater emphasis has been placed upon the application of computers to the social sciences, and much less upon original contributions in the areas of interest of the first workers on automatic computers. The second difference was in the composition of the Symposium: the others were attended by hundreds of participants from all over the world; 47 people met informally on this occasion and all but a handful of these were Faculty members of Harvard itself. Accordingly, this must have been a much more domestic affair than the earlier ones, and inevitably has sacrificed something of the authority of the earlier Symposia. The variety of topics is so great that it is unlikely that many of such a small gathering fully understood all the papers, or even that many would do so for any particular paper; the reviewer is certainly in no

better position than those attending and he, therefore, cannot comment on all the papers.

Several of the contributions were surveys of possible and actual computer applications in special fields. These papers will be full of interest to someone outside such fields, and yet give valuable guidance and will be a source of useful references for those workers thinking of applying computers to similar problems. The papers on computers in Educational Research, Public Health, X-Ray Crystallography, Medicine, Statistics, Economics, Psychological Research and Business Administration were of this type. Some of the problems mentioned required the application of known techniques—for example, statistical ones—but have awaited the simultaneous occurrence of the right equipment and the right investigator. Other problems posed are those of what E. B. Newman calls paracomputation—non-computational uses of computers. If a criticism is to be levelled here it is that much of what is written is too imprecise to tell a reader how he should proceed on his own machine. Simulation is featured in several papers; one on Queueing Theory and Reservoir Design gives numerical examples of the calculations performed.

There are several papers which show the sorts of differential equations which arise in physical problems, and the numerical methods available for their solution. Examples are given from hydrodynamics, plasma dynamics, kinetics and molecular-beam theory.

Two of the longest papers in the volume deal with document content, one in the context of information retrieval, and the other, by Mosteller and Wallace, about the problem of disputed authorship. The latter work received considerable publicity in the American press because of the great public interest in all matters pertaining to the Constitution. The problem was to determine which of Alexander Hamilton and James Madison wrote certain papers urging the ratification of the Constitution. Even to an Englishman this paper contains a fascinating account of the work by two eminent statisticians to clarify the obscurity of history. They describe the early work, how one of them thought it easy but long, how wives and others counted, how checks were necessary, how first ideas failed to give any indications to the answer, and how finally computer counts yielded data to which their statistical methods might be applied and so point to a conclusive answer.

The editor, who has himself contributed a paper with the intriguing title: "The Geometry of Symbols", is to be congratulated on disciplining his colleagues to such an extent that their accounts only rarely seem to become incomprehensible—a considerable achievement when dealing with material of such interesting diversity. E. S. PAGE