A mechanization of algebraic differentiation and the automatic generation of formulae for molecular integrals of Gaussian orbitals

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A simple representation of complicated functions of many variables is described. Methods are given for forming automatically partial derivatives of any order, and it is shown how symmetry may be exploited to achieve compactness of representation. These methods have been used extensively in the generation of formulae for molecular integrals of Gaussian orbitals in a form suitable for subsequent evaluation in calculations of molecular structure.

1. Introduction

The present investigation arose from the need to evaluate as accurately as possible large numbers of partial derivatives, of various orders, of functions which were themselves quite complicated expressions in up to sixteen arguments. A numerical approach using finite differences was rejected on grounds of accuracy, speed and storage limitations. As for analytical differentiation by hand, the magnitude of the task and the difficulty of checking the results proved a sufficient deterrent. Automatic differentiation by electronic computer was the only feasible method.

Other work on automatic differentiation that has been reported mostly uses symbolic or list-processing languages. McCarthy (1960) gives a simple example of a differentiation program in LISP, and a more complete treatment is given by Cooper (1961) using ALP. A comprehensive treatment is given by Hanson, Caviness and Joseph (1962). The work now described was begun on an Elliott 402 computer by kind permission of I.C.I. Ltd., and was continued subsequently on the Ferranti Pegasus at Leeds University. In both cases it was necessary to use machine-language coding; such autocodes as were available were not suited to problems in symbol manipulation. A dominant feature is the emphasis on the subsequent applications of the results that are obtained. A new approach is given to the way in which the functions to be differentiated are represented. The conventional algebraic symbolism is reduced to the form of a numerical array which permits of convenient and efficient manipulation both for differentiation and evaluation.

In Section 2 we review the context in which the investigation was begun. A full account of the mathematical stages in a quantum-mechanical calculation of molecular structure has been given by Boys and Cook (1960). The exact solution is approximated by a finite expansion in functions selected from a complete system. The functions used in the investigation were of Gaussian form characterized by an exponential radial factor $\exp(-\alpha r_A^2)$ where α is a positive parameter and r_A denotes distance from an atomic nucleus at a point A. It was shown by Boys (1950) that in such a basis all the integrals can be evaluated from closed formulae. The present paper is concerned with the automatic generation of these formulae.

In Section 3 we describe the representation of a function by a multinomial expansion having as arguments a set of auxiliary functions. By careful choice of the auxiliary functions, the set of multinomials is closed under differentiation. Derivatives of any order may thus be obtained by simple iteration. Section 4 reviews the elementary processes for the analytical differentiation of an algebraic expression. A key problem in automatic differentiation is the simplification of the expressions that result from applying these processes.

The representation of functions by multinomials permits a great deal of simplification of the derivatives to be obtained quite naturally and conveniently. In Section 5 it is shown how in certain cases simultaneous rather than sequential application of a pair of differential operators can lead to a still more compact representation of a second-order derivative. A brief discussion of the evaluation of the multinomials and of the estimation of the associated rounding errors is given in Section 6.

2. Molecular integrals of Gaussian orbitals

An *orbital* is the name given to a function of the positional co-ordinates of an electron in physical space. Those that we shall consider are of Gaussian form,

$$\eta(A, a, \alpha, r) = x_A^{a_1} y_A^{a_2} z_A^{a_3} r_A^{2a_4} \exp(-\alpha r_A^2)$$

where $r = (x, y, z)$ is the position vector of the electron in rectangular Cartesian co-ordinates, $A = (A_x, A_y, A_z)$ is the position vector of an atomic nucleus, $a = (a_1, a_2, a_3, a_4)$ are positive or zero integer parameters, and α is a positive constant. We have written x_A for for $(x - A_x)$, etc., and $r_A^2 = x_A^2 + y_A^2 + z_A^2$.

The integrals that are needed in a molecular wave-function calculation are the single-electron integrals

$$I = \int \eta(A, a, \alpha, r) K \eta(B, b, \beta, r) dV$$

and the two-electron electrostatic integrals

$$I = \int\int \eta(A, a\ \alpha, r_1)\eta(B, b, \beta, r_1)\frac{1}{r_{12}} \eta(C, c, \gamma, r_2)\eta(D, d, \delta, r_2)dV_1dV_2$$

where the volume elements are at the positions of the electrons, and the integrations are over all space. There are various classes of single-electron integral corresponding to different operators K; overlap integrals have $K = 1$, kinetic energy integrals have $K = -\frac{1}{2}\nabla^2$, where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is the Laplacian operator, and the nuclear potential integrals have $K = 1/r_F$, where F is the position vector of an atomic nucleus.

Formulae for these integrals may all be obtained systematically. It is easily shown that

$$P(a_4|a_4 + 1)\eta(A, a, \alpha, r) = -\frac{\partial}{\partial\alpha}\eta(A, a, \alpha, r)$$

and that if $a_4 = 0$,

$$P(a_1|a_1 + 1)\eta(A, a, \alpha, r) = \frac{1}{2\alpha}\left\{\frac{\partial}{\partial A_x} + a_1P(a_1|a_1 - 1)\right\}\eta(A, a, \alpha, r), \text{ etc.}$$

In these expressions $P(u|v)$ denotes a substitution operator which replaces u by v in the expression which follows it. Thus for any function $\phi(u)$,

$$P(u|v)\phi(u) = \phi(v).$$

For any of the integrals, I, it follows that, for $a_4 = 0$,

$$I(a_1 + 1) = \frac{1}{2\alpha}\frac{\partial}{\partial A_x}I(a_1) + \frac{a_1}{2\alpha}I(a_1 - 1), \text{ etc.}$$

and for general a_4,

$$I(a_4 + 1) = -\frac{\partial}{\partial\alpha}I(a_4).$$

Similar results are valid for the centres B, C and D, and the respective parameters (b, β), (c, γ) and (d, δ).

The formula for any combination of indices a, b, c, d can thus be generated from that corresponding to all zero indices by applying first sufficient relations of the first type and then sufficient of the second type. The relevant basic formulae are given by Boys (1950).

$$\int e^{-\alpha r_A^2 - \beta r_B^2}dV = \left(\frac{\pi}{\alpha+\beta}\right)^{3/2}\exp\left(-\frac{\alpha\beta}{\alpha+\beta}AB^2\right)$$

$$\int e^{-\alpha r_A^2}(-\tfrac{1}{2}\nabla^2)e^{-\beta r_B^2}dV = \left\{3\left(\frac{\alpha\beta}{\alpha+\beta}\right) - 2\left(\frac{\alpha\beta}{\alpha+\beta}\right)^2AB^2\right\} \times \left(\frac{\pi}{\alpha+\beta}\right)^{3/2}\exp\left(-\frac{\alpha\beta}{\alpha+\beta}AB^2\right)$$

$$\int e^{-\alpha r_A^2 - \beta r_B^2}\frac{1}{r_F}dV = \frac{2\pi}{\alpha+\beta}\exp\left(-\frac{\alpha\beta}{\alpha+\beta}AB^2\right)\mathscr{F}[(\alpha+\beta)EF^2]$$

$$\int\int e^{-\alpha r_{1A}^2 - \beta r_{1B}^2}\frac{1}{r_{12}}e^{-\gamma r_{2C}^2 - \delta r_{2D}^2}dV_1dV_2 = \frac{2\pi^{5/2}}{(\alpha+\beta)(\gamma+\delta)(\alpha+\beta+\gamma+\delta)^{1/2}}\exp\left(-\frac{\alpha\beta}{\alpha+\beta}AB^2 - \frac{\gamma\delta}{\gamma+\delta}CD^2\right)\mathscr{F}\left[\frac{(\alpha+\beta)(\gamma+\delta)}{(\alpha+\beta+\gamma+\delta)}EF^2\right]$$

where

$$E = (\alpha A + \beta B)/(\alpha + \beta),\ F = (\gamma C + \delta D)/(\gamma + \delta)$$

and

$$\mathscr{F}(x) = \int_0^1 e^{-xt^2}dt.$$

The use of the vector F in two different contexts is deliberate in order to unify nomenclature for the analysis of the various classes of integral. In practice no confusion can arise.

The formula for general indices a, b, c, d is thus ultimately expressible in terms of the corresponding basic formula above and various of its partial derivatives of various orders with respect to the parameters A, α, B, β, C, γ, D, δ.

3. A multinomial representation

The representation chosen for each formula in the computer was a multinomial expansion in terms of a pre-assigned set of auxiliary functions. Thus we write the function $f(t)$ as

$$f(t) = \sum_i C_i \prod_j x_j^{u_{ij}}$$

where $x_j(t)$ are a finite set of auxiliary functions of t. This may be stored in the machine as an array of indices u_{ij} and an array of coefficients C_i.

The derivatives of f with respect to t may be written as

$$f'(t) = \sum_i C_i \sum_k x_k'u_{ik}P(u_{ik}|u_{ik} - 1)\prod_j x_j^{u_{ij}}.$$

Now by careful choice of the auxiliary functions it is possible in our application—and presumably in general—to arrange that the derivatives x_k' are each expressible as multinomials of the same set of auxiliary functions

$$x_k' = \sum_i D_{kl}\prod_j x_j^{v_{jk}}.$$

The first derivative of f can thus similarly be expressed as a multinomial expansion in the same set of auxiliary functions by substitution of the non-trivial x_k' in the above expression for $f'(t)$. Carrying out this substitution is the basis of the computer program for differentiation. The only simplification of the resulting expansion which needs to be made is to compare the various products $C_i\prod_j x_j^{u_{ij}}$ against each other after production, so that any two which have the same $\prod_j x_j^{u_{ij}}$ can be condensed by adding their coefficients C_i. Derivatives of any higher order may be obtained by iteration. The auxiliary functions are chosen to be of the simplest possible form

Table 1

The auxiliary functions

j	x_j	j	x_j
0	$A_x - B_x$	18	$E_z - F_z$
1	$A_y - B_y$	19	EF^2
2	$A_z - B_z$	20	$(A - B).(E - F)$
3	AB^2	21	$(C - D).(E - F)$
4	2α	22	$(A - B).(C - D)$
5	2β	23	$[2(\alpha + \beta + \gamma + \delta)]^{1/2}$
6	$[2(\alpha + \beta)]^{1/2}$	24	$\mathscr{F}\left[\frac{(\alpha + \beta)(\gamma + \delta)}{(\alpha + \beta + \gamma + \delta)} EF^2\right]$
7	$k \exp\left(-\frac{\alpha\beta}{\alpha + \beta} AB^2\right)$	25	$\mathscr{F}'\left[\frac{(\alpha + \beta)(\gamma + \delta)}{(\alpha + \beta + \gamma + \delta)} EF^2\right]$
8	$C_x - D_x$	26	$\mathscr{F}''\left[\frac{(\alpha + \beta)(\gamma + \delta)}{(\alpha + \beta + \gamma + \delta)} EF^2\right]$
9	$C_y - D_y$	27	$\mathscr{F}'''\left[\frac{(\alpha + \beta)(\gamma + \delta)}{(\alpha + \beta + \gamma + \delta)} EF^2\right]$
10	$C_z - D_z$	28	$\mathscr{F}''''\left[\frac{(\alpha + \beta)(\gamma + \delta)}{(\alpha + \beta + \gamma + \delta)} EF^2\right]$
11	CD^2	29	$\mathscr{F}[(\alpha + \beta)EF^2]$
12	2γ	30	$\mathscr{F}'[(\alpha + \beta)EF^2]$
13	2δ	31	$\mathscr{F}''[(\alpha + \beta)EF^2]$
14	$[2(\gamma + \delta)]^{1/2}$	32	$2(\alpha - \beta)$
15	$\exp\left(-\frac{\gamma\delta}{\gamma + \delta} CD^2\right)$	33	$2(\gamma - \delta)$
16	$E_x - F_x$	34	$4(\alpha^2 + \beta^2)$
17	$E_y - F_y$	35	$4(\gamma^2 + \delta^2)$

so that the x'_k may be formed by hand on inspection, and fed into the machine in coded form. The scheme is readily extended to the generation of partial derivatives of functions of several arguments. In this case it is necessary to furnish a list x'_k for differentiation with respect to each argument.

In order that the formulae obtained should be represented exactly in the machine, all the indices and coefficients are restricted to be of type integer. To this end it is often necessary to absorb a constant factor into some of the auxiliary functions. For greater administrative convenience the auxiliary functions appropriate to each class of integral are gathered together into one common set. This is shown in Table 1. The members of the set are not independent, and simplification of the formulae is thereby made more difficult. This problem is considered further in the next section.

Clearly the set is not unique. The set listed is in fact restrictive in its treatment of the function $\mathscr{F}$ and its derivatives. In the evaluation of the formulae a procedure was used which computed $\mathscr{F}(x)$ and appropriate derivatives effectively in a single operation. The range of formulae currently in use is that derived from the restricted set of orbitals

$$e^{-\alpha r_A^2},\ x_A e^{-\alpha r_A^2},\ y_A e^{-\alpha r_A^2},\ z_A e^{-\alpha r_A^2},\ r_A^2 e^{-\alpha r_A^2}.$$

The auxiliary functions of Table 1 are thus adequate in that there is no occasion to make use of the derivatives of x_{28} or x_{31}. It will be necessary to reconsider this choice when calculations are extended to other orbitals on a more powerful machine.

The basic formulae are now readily expressed in terms of the auxiliary functions. As example, that for the two-electron electrostatic integral is

$$+1x_6^{-2}x_7^{+1}x_{14}^{-2}x_{15}^{+1}x_{23}^{-1}x_{24}^{+1}$$

where the constant k absorbed into x_7 is $2(2\pi)^{5/2}$.

A further illustration is provided by the expressions for $\frac{1}{2\alpha}\frac{\partial}{\partial A_x}x_k$ in Table 2. Only the non-zero entries are

given explicitly. Hence, for example, we may operate with this operator on the basic formula above to produce the higher formula for

$$\iint x_{1A} e^{-\alpha r_{1A}^2 - \beta r_{1B}^2} \frac{1}{r_{12}} e^{-\gamma r_{2C}^2 - \delta r_{2D}^2} \, dV_1 dV_2$$

viz.: $-1x_0^{+1}x_5^{+1}x_6^{-4}x_7^{+1}x_{14}^{-2}x_{15}^{+1}x_{23}^{-1}x_{24}^{+1}$
$+1x_6^{-2}x_7^{+1}x_{15}^{+1}x_{16}^{+1}x_{23}^{-3}x_{25}^{+1}.$

4. The elementary rules for differentiation

Simple rules for differentiation are of the following types,

$$(f+g)' = f' + g'$$
$$(fg)' = f'g + fg'$$
$$(f^n)' = nf^{n-1}f'$$
$$\{f(g)\}' = \left\{\frac{d}{dg}f(g)\right\}g'.$$

The differentiation of an actual expression involves repeated application of such rules. A number of purely algebraic rules must also be applied in order to simplify the resulting expressions. Typical of these are,

$$f + 0 = f$$
$$f \times 0 = 0$$
$$f \times 1 = f$$
$$f \,/\, f = 1$$
$$f - f = 0$$
$$f + f = 2f.$$

Other sources of simplification are more difficult to detect and apply. Thus, for example,

$$\cos^2\theta + \sin^2\theta = 1$$
$$\log_e(\exp f) = f$$
$$2\cosh f = e^f + e^{-f}$$
$$r^2 = x^2 + y^2 + z^2.$$

It is of prime importance that the expression resulting from a computer program be as simple as possible. The expression is only generated once but may be used many times for evaluation. An economic representation should take care of the application of as many of the above rules as possible. The representation as a list of algebraic symbols is highly uneconomic as every type of redundancy mentioned above can occur, and further routines must be introduced to search for and remove them. A glance at the output from McCarthy's (1960) program will confirm this. Furthermore, it is important that all the simple rules for differentiation are included. Thus Cooper (1961) makes no provision for exponentiation. The function x^3 is represented as $x \times x \times x$, and its derivative with respect to x as $(x \times x) + (x \times x) + (x \times x)$. Functions with fractional powers become even more tortuous to operate upon. It is difficult to remove any but the simplest kinds of redundancy from expressions represented in this way.

The representation described in Section 3, however, accounts naturally for most of the simple kinds of redundancy through its implementation as a set of numerical arrays. Only the last two forms of simple redundancy can occur, and these can be detected by comparing the terms in an expansion one against the other.

Table 2

Multinomial expressions for $\frac{1}{2\alpha}\frac{\partial}{\partial A_x}x_k$

$k =$ 0	$+1x_4^{-1}$
3	$+2x_0^{+1}x_4^{-1}$
7	$-1x_0^{+1}x_5^{+1}x_6^{-2}x_7^{+1}$
16	$+1x_6^{-2}$
19	$+2x_6^{-2}x_{16}^{+1}$
20	$+1x_4^{-1}x_{16}^{+1} +1x_0^{+1}x_6^{-2}$
21	$+1x_6^{-2}x_8^{+1}$
22	$+1x_4^{-1}x_8^{+1}$
24	$+1x_{14}^{+2}x_{16}^{+1}x_{23}^{-2}x_{25}^{+1}$
25	$+1x_{14}^{+2}x_{16}^{+1}x_{23}^{-2}x_{26}^{+1}$
26	$+1x_{14}^{+2}x_{16}^{+1}x_{23}^{-2}x_{27}^{+1}$
27	$+1x_{14}^{+2}x_{16}^{+1}x_{23}^{-2}x_{28}^{+1}$
29	$+1x_{16}^{+1}x_{30}^{+1}$
30	$+1x_{16}^{+1}x_{31}^{+1}$

A further consideration is the effect of rounding errors on the results of evaluating the formulae. If the expressions are highly redundant, such that two large equal and opposite terms are present, then the effect on the accuracy of the final result might be disastrous. A check was kept on the accuracy of all integrals evaluated from the formulae produced by this method, and a high degree of accuracy was always in evidence.

5. Symmetric differentiation

The representation of functions by multinomials permits a considerable simplification of derived expressions to be made almost trivially. Recognition of like terms in a lengthy expression is time consuming but presents no essential difficulty. Any term whose net coefficient is found to be zero is removed from the expansion.

The scheme as described was satisfactory except that certain of the derived formulae were rather long and clumsy. This stems from the failure to recognize the existence of functional relationships amongst the auxiliary functions. Thus, for example, in terms of auxiliary functions α, β and $(\alpha + \beta)$ one might have

$$f = \alpha\beta(\alpha + \beta)^{-1},$$

so that

$$\frac{\partial}{\partial\alpha}f = \beta(\alpha + \beta)^{-1} - \alpha\beta(\alpha + \beta)^{-2}$$

and

$$\frac{\partial}{\partial\beta}\frac{\partial}{\partial\alpha}f = (\alpha+\beta)^{-1} - \beta(\alpha+\beta)^{-2} - \alpha(\alpha+\beta)^{-2} + 2\alpha\beta(\alpha+\beta)^{-3}.$$

No simplification is possible with the basic scheme, but if there were some means of combining the middle two terms into $-(\alpha+\beta)^{-1}$, this would be cancelled with the first term leaving

$$\frac{\partial^2 f}{\partial\alpha\partial\beta} = 2\alpha\beta(\alpha+\beta)^{-3}.$$

It was found uneconomic to inspect for common factors of groups of terms in this way, but a similar simplification was achieved by a technique of simultaneous symmetric differentiation. The basis of the method is to arrange that if a function has a certain symmetry, it is represented solely in terms of auxiliary functions having the same symmetry.

If G and H are two differential operators, then the result of sequential operation on the general term $\prod_j x_j^{u_j}$ is

$$\begin{aligned} GH\prod_j x_j^{u_j} &= G\Big\{\sum_k (Hx_k)u_k P(u_k|u_k-1)\prod_j x_j^{u_j}\Big\} \\ &= \sum_k (GHx_k)u_k P(u_k|u_k-1)\prod_j x_j^{u_j} \\ &\quad + \sum_{k,l}(Gx_l)(Hx_k)u_l P(u_l|u_l-1) \\ &\qquad \Big\{u_k P(u_k|u_k-1)\prod_j x_j^{u_j}\Big\}. \end{aligned}$$

Now in the double summation the factors of $(Hx_k)(Gx_l)$ and $(Hx_l)(Gx_k)$ are the same. We can therefore derive a symmetric form suitable for programming:

$$\begin{aligned} GH\prod_j x_j^{u_j} &= \sum_k S_k u_k P(u_k|u_k-1)\prod_j x_j^{u_j} \\ &\quad + \sum_{k\geqslant l} T_{kl}u_l P(u_l|u_l-1)\Big\{u_k P(u_k|u_k-1)\prod_j x_j^{u_j}\Big\} \end{aligned}$$

where $S_k = GHx_k$

and $$T_{kl} = \begin{cases}(Gx_k)(Hx_l)+(Gx_l)(Hx_k) & \text{if } k\neq l\\ (Gx_k)(Hx_k) & \text{if } k=l.\end{cases}$$

Suppose that the auxiliary functions x_j present in the term $\prod_j x_j^{u_j}$ above are each invariant under some permutation of arguments which interchanges G and H. Now G and H are differential operators and therefore commute. It follows that each of S_k and T_{kl} are invariant under this permutation, and we shall suppose that each is expressed as a multinomial in terms of auxiliary functions which are similarly invariant. Finally, we see that $GH\prod_j x_j^{u_j}$ has this same symmetry and is expressed, after substitution for the S and T elements, as a multinomial in terms of auxiliary functions which also have this symmetry.

To summarize, the non-symmetric sequential operations "H then G" are replaced by the symmetric simultaneous operations S and T. From symmetry considerations, therefore, a more compact formula is produced.

Continuing the example above, we write $x_0 = \alpha\beta$, $x_1 = \alpha+\beta$ and take $G = \frac{\partial}{\partial\alpha}$, $H = \frac{\partial}{\partial\beta}$ noting that x_0 and x_1 are symmetric in α and β. We then have

$$\begin{aligned} S_0 &= 1 & T_{00} &= x_0 \\ S_1 &= 0 & T_{10} &= x_1 \qquad T_{11} = 1, \end{aligned}$$

so that

$$\begin{aligned} \frac{\partial^2}{\partial\alpha\partial\beta}\alpha\beta(\alpha+\beta)^{-1} &= GHx_0x_1^{-1} \\ &= S_0x_1^{-1} + T_{00}\cdot 0 \\ &\qquad + 2T_{11}x_0x_1^{-3} + T_{10}(-x_1^{-2}) \\ &= x_1^{-1} + 2x_0x_1^{-3} - x_1^{-1} \\ &= 2x_0x_1^{-3} \\ &= 2\alpha\beta(\alpha+\beta)^{-3}. \end{aligned}$$

In order to apply this technique to the molecular integrals, we note that each of the basic formulae quoted in Section 2 is invariant under interchange of the sets A, α with B, β, and similarly with respect to the sets C, γ and D, δ. We therefore arrange to represent them in terms of auxiliary functions with the same property—see, for example, the representation quoted in Section 4 for the two-electron electrostatic integral. Symmetric differentiation may thus be used for applying the operators

$$\frac{\partial^2}{\partial A_x\partial B_x},\ \frac{\partial^2}{\partial A_y\partial B_y},\ \frac{\partial^2}{\partial A_z\partial B_z},\ \frac{\partial^2}{\partial\alpha\partial\beta}$$

and a similar set derived from C, and D. The technique was extremely successful; the longest formula produced, that for

$$\iint r_{1A}^2 r_{1B}^2 e^{-\alpha r_{1A}^2-\beta r_{1B}^2}\frac{1}{r_{12}}r_{2C}^2 r_{2D}^2 e^{-\gamma r_{2C}^2-\delta r_{2D}^2}dV_1dV_2$$

being reduced from some eight hundred terms to about three hundred.

To apply this method to best advantage it is necessary to produce the expressions for S_k and T_{kl} in the simplest form. This can usually be done, again by hand, on inspection. Although extra work is needed to prepare the derivatives this again has to be done only once, whereas the economy in the formula is exploited every time that it is used for evaluation.

6. The evaluation of the formulae

This account would not be complete without some reference to the evaluation of the formulae. A typical molecular wavefunction calculation may require the evaluation of several thousand integrals employing over a hundred different formulae. It is thus important that evaluation should be efficient, though fortunately, the majority of the integrals are evaluated from the shorter formulae.

The data for an evaluation are the numerical values of the orbital parameters A, α, etc. The first stage of the calculation is the evaluation of all the auxiliary functions, it not being thought worthwhile to program the selection only of those required for the particular integral. Similarly no attempt was made to carry over the values of any of the auxiliary functions from one integral to another.

The successive terms of the multinomial were then evaluated and their sum accumulated. At this stage a check on the accuracy of the evaluation was carried out. All arithmetic was in the floating-point mode with a binary exponent and a nominal precision of 38 significant binary digits. The maximum exponent over all terms and over all partial sums was recorded. The excess of this over the exponent of the final result is a measure of the differencing error incurred. Numerous evaluations have suggested that this error does not amount to more than two or three binary digits.

In the evaluation of each term $C\prod_j x_j^{u_j}$ the array u was scanned and zero entries ignored. The remaining factors were formed by using the digits of the binary representation of mod(u_j) to select contributions from the sequence obtained by repeatedly squaring x_j or $1/x_j$. Each term was evaluated independently of the rest. Were it not for the limited rapid-access storage available on the machines used, it might have been worthwhile preserving some information from one term to the next. Thus the sequence x_j, x_j^2, x_j^4, ... might have been preserved. For $u_j > 0$, $x_j^{u_j}$ would have been calculated as a product of selections from this sequence as before; for $u_j < 0$ then $1/x_j^{-u_j}$ would have been calculated. The terms of the sequence would best be calculated when first required; the number of terms currently available could be stored and the sequence could readily be extended as needed.

It is thought that the speed of evaluation could be significantly increased on suitable machines in this way. There are, however, further improvements which are theoretically possible and which would be very rewarding if means could be devised for implementing them automatically. The simplest example is the insertion of brackets in the expression for a polynomial prior to evaluating it by nested multiplication thus:

$$ax^3 + bx^2 + cx + d = ((ax + b)x + c)x + d.$$

Still more efficient means of evaluating polynomials are discussed by Knuth (1962). The present paper shows how general functions of several variables may be reduced to multinomials, albeit with some loss of efficiency due to unexploited dependency among the auxiliary functions. Even in this limited field, however, there appears to be no theoretical treatment of the evaluation problem. Any proposal, to be useful in the present context, must be capable of evaluating efficiently an expression whose precise form is not known to the programmer. This is, of course, a much greater problem than that posed by the evaluation of any particular expression, however complex.

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