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Note

A Numerical Differentiator

1. INTRODUCTION

It is considered wise to avoid numerical differentiation wherever possible because the very nature of the problem can induce numerical cancellation and the result is relatively low accuracy in the derivative values (Hildebrand [1]). However, in some physical problems numerical differentiation is difficult to avoid completely while in others derivatives appear, but their direct evaluation is usually avoided by suitable reformulation. Such a problem arose in the numerical technique of (Blakemore, Evans and Hyslop [3], [4]) for solving the Hartree–Fock equations for a general atom. The iterated wave functions at each stage are represented as tables of values, very much in the spirit of Hartree's original work [8]. However in the present context the tabular points are chosen to be the cosine weighted abscissas of the Clenshaw–Curtis quadrature formula [5] on a set of subintervals. The number of abscissas in each subinterval was chosen to yield the required accuracy and the integrations (both definite and indefinite) could be performed using just these tabulated values. Furthermore the subintervals extended until the contribution from the integrands had fallen off sufficiently to be neglected. In this way the infinite range was handled, and any regions in which the integrands varied rapidly could have a concentration of abscissas.

The Hartree–Fock equations in general involve Lagrange multipliers λ_{ij} which need to be evaluated as part of the above scheme. It was decided to investigate the use of the direct evaluation of the formula

$$-N_j\lambda_{ij} = \int_0^\infty P_j(r)\left[-\frac{1}{2}\frac{d^2}{dr^2} - \frac{Z}{r} + \frac{l_i(l_i+1)}{r^2}\right]P_i(r)\,dr + I \qquad (1)$$

where N_j is the number of electrons in the jth. orbital, P_i and P_j are the r-weighted wave functions in the ith and jth orbitals respectively, Z is the atomic number, l_i is the l-quantum number for the orbital and I is an integral which can be treated directly. The form (1) is only needed in atoms which have different orbitals with equal numbers of electrons and whose l-quantum numbers are the same. The λ_{ij}'s are then used when applying the Roothaan procedure [6], which deals with the non-pseudo-eigenvalue form of the Hartree-Fock equations. Alternative procedures are available for this problem which avoid numerical differentiation, but the direct approach may be more generally applicable to other integral and integro-differential equations where alternatives are not possible. Hence a direct numerical approach was investigated in this problem.

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Integration of (1) by parts shows that integrals of the form

$$\int_0^\infty \frac{dP_i}{dr}\frac{dP_j}{dr}\,dr \tag{2}$$

are required in which the functions P_i and P_j are known at tabulated points. Clearly, with this approach, a numerical differentiation procedure is required for these terms which has the property that errors may be continuously monitored during the computation in the same way as in the numerical integration method. Form (2) is used in preference to (1) as the second order derivatives are not obtained as a by-product of other calculations as in some conventional approaches, but need to be found from the wave functions. In this situation errors are reduced by having only first order derivatives to find.

2. The Differentiation Formula

Consider a function $f(x)$ which is tabulated on a particular subinterval [a, b]. Then the function $F(t)$ given by

$$F(t) = f\left(\frac{b-a}{2}\,t + \frac{b+a}{2}\right) \tag{3}$$

is defined on the interval $[-1, 1]$ and the usual Chebyshev expansion yields

$$F(t) = \sum_{i=0}^{M\prime} a_i T_i(t) + E(t) \tag{4}$$

where

$$a_i = \frac{2}{M}\sum_{s=0}^{M\prime\prime} f\left(\cos\frac{\pi s}{M}\right)\cos\frac{\pi i s}{M}, \tag{5}$$

$$T_i(t) = \cos(i\cos^{-1}t), \tag{6}$$

$E(t)$ is the error term, $\sum'$ denotes the first term is halved and $\sum''$ denotes that the first and last terms are halved (Clenshaw and Curtis [5]).

The derivative can be written as

$$\frac{df}{dx} = \frac{2}{(b-a)}\frac{dF}{dt} \sim \frac{2}{(b-a)}\sum_{i=1}^{M} a_i T_i'(t)$$

$$= \frac{2}{(b-a)}\sum_{i=1}^{M} a_i i \sin i\theta/\sin\theta \tag{7}$$

where $\theta = \cos^{-1}t$ and $x = \frac{1}{2}(b+a) + \frac{1}{2}(b-a)t$.

In the case when the derivative is required at the cosine weighted points $x_s = (b - a)/2 \cos(\pi s/M) + (b + a)/2$ then $\theta_s = \pi s/M$ and the formula reduces to

$$\frac{df}{dx}\Big|_{x_s} = \frac{2}{(b-a)} \sum_{i=1}^{M} a_i i \sin \frac{\pi i s}{M} \Big/ \sin \frac{\pi s}{M} \tag{8}$$

Hence a table of values is generated which has immediate application in a Clenshaw–Curtis quadrature routine to evaluate (2). For wider applications the more general formula (7) would be employed.

3. Errors

If we write for the infinite expansion

$$F(t) = {\sum_{i=0}^{\infty}}' A_i T_i(t) \tag{9}$$

then it was shown by Clenshaw and Curtis and again by O'Hara and Smith [7] that the coefficients for the finite expansion are given by

$$a_i = A_i + \sum_{j=1}^{\infty} (A_{2jM-i} + A_{2jM+i}) \tag{10}$$

Then the error $E'(t)$ in dF/dt is given by:

$$E'(t) = -\sum_{i=1}^{M} \left[\sum_{j=1}^{\infty} (A_{2jM-i} + A_{2jM+i}) \right] T_i'(t) + \sum_{i=M+1}^{\infty} A_i T_i'(t) \tag{11}$$

The coefficients A_j fall off as K_M/j_p for $j \geqslant M$ where $(p - 1)$ is the order of the first discontinuous derivative of $f(t)$ and K_M is a constant independent of j. For example a function with a continuous first derivative but a discontinuous second derivative has a fall off like K_M/j^3 (O'Hara and Smith [7]) which will be the most slowly converging case it will be necessary to consider here. It then follows that computational approximations

$$A_M = a_M/2 \qquad \text{and} \qquad A_{M-i} = a_{M-i} \tag{12}$$

can be adopted to estimate the A's for use in an error estimate of the O'Hara and Smith variety.

The error formula for $E'(t)$ may be re-grouped in terms of ascending coefficients in the form

$$\begin{aligned} E'(t) = &-A_M T'_M(t) + A_{M+1}[T'_{M+1}(t) - T'_{m-1}(t)] + \cdots + A_{2M-1}[T'_{2M-1}(t) - T'_1(t)] \\ &+ A_{2M}T'_{2M}(t) + A_{2M+1}[T'_{2M+1}(t) - T'_1(t)] + \cdots + A_{3M}[T'_{3M}(t) - 2T'_M(t)] \\ &+ A_{3M+1}[T'_{3M+1}(t) - T'_{M-1}(t)] + \cdots + A_{4M-1}[T'_{4M-1}(t) - T'_1(t)] \\ &+ A_{4M}T'_{4M}(t) + A_{4M+1}[T'_{4M+1}(t) - T'_1(t)] + \cdots \\ &+ A_{5M}[T'_{5M}(t) - 2T'_M(t)] + \cdots . \end{aligned} \tag{13}$$

Applying the inequality

$$T'_j(t) = \frac{j \sin j\theta}{\sin \theta} \leqslant j^2 \qquad \text{where} \quad t = \cos \theta \tag{14}$$

and using the relation

$$| T'_{M+i}(t) - T'_{M-i}(t)| = \left| \frac{2i \cos i\theta \sin m\theta + 2m \cos m\theta \sin i\theta}{\sin \theta} \right| \leqslant 4mi \tag{15}$$

yields

$$\begin{aligned} | E'(t)| < \{&M^2 | A_M | + 4M | A_{M+1} | + 8M | A_{M+2} | + \cdots + 4M(M-1) | A_{2M-1}| \\ &+ | A_{2M} | 4M^2 - \cdots\} \end{aligned} \tag{16}$$

Hence if the A_M's fall off sufficiently quickly then

$$| E'(t)| \sim K_M/M^{p-2} \tag{17}$$

The upper bound on $T'_j(t)$ occurs at the end points where the worst error is to be expected. The best error in the range will be of order $1/M$ times the worst.

In order to make a dynamic estimate of the error in the programme, assume the form (17) and use (12) to give

$$K_M \sim A_M M^p \tag{18}$$

and

$$| E'(t)|^2 = A_M M^2 = a_M M^2/2 \tag{19}$$

which gives a simple error estimate.

This error estimate appears to give the order of the error successfully in the examples considered in the next paragraph.

4. Results and Conclusions

Testing was carried out firstly on the function

$$cxe^{-cx}$$

for a range of $c = (0.5, 1.0, 2.0, 4.0, 8.0)$ on the interval $x \in [0, 1]$. The larger c the steeper is the curve being considered. This function has physical significance in the underlying application which initiated this work in that the function is a Slater function for atomic orbitals with quantum number $l = 1$. As a comparison a conventional finite difference formula in Lagrangian form was applied to the problem with the same number of points (now equally spaced). Formulae of orders $M = 5, 10, 15, 20$ were used on each c value. The actual absolute errors from both the Chebyshev method and the finite difference method, together with the above estimates of the Chebyshev error were tabulated over a range of 20 points in the interval of interest. The errors varied from the largest values at the end points to the best values at the middle of the range, as would be expected from (14) for the Chebyshev case. This effect was particularly marked in the finite difference errors, the Chebyshev errors usually giving a more uniform spread. However the finite difference method suffers much more severe loss of accuracy than the Chebyshev method at these end point regions. It appears

TABLE I

Chebyshev and Lagrangian Absolute Errors for $f'(x)$ on [0, 1] where $f(x) = cxe^{-cx}$ with an $(M + 1)$ Point Formula

C	M	Actual Chebyshev error at 0	Actual Lagrange error at 0	Actual Chebyshev error at 1	Actual Lagrange error at 1	Actual Chebyshev error at $\frac{1}{2}$	Actual Lagrange error at $\frac{1}{2}$	Estimated truncation error
0.5	5	9.2(−5)	3.9(−6)	9.6(−5)	3.6(−6)	1.7(−5)	2.3(−7)	9.4(−5)
	10	8.7(−11)	7.3(−10)	2.6(−9)	4.4(−9)	4.7(−11)	1.5(−10)	1.1(−10)
	15	1.0(−9)	3.5(−8)	5.4(−9)	4.5(−8)	1.1(−10)	3.2(−10)	1.7(−10)
1.0	5	2.2(−3)	2.0(−4)	2.3(−3)	1.6(−4)	4.2(−4)	1.1(−5)	2.2(−3)
	10	4.9(−10)	2.5(−9)	3.0(−9)	4.9(−9)	1.2(−10)	1.1(−10)	4.5(−10)
	15	6.4(−10)	6.8(−8)	1.1(−8)	1.0(−8)	1.5(−10)	4.3(−10)	4.7(−10)
2.0	5	3.7(−2)	7.8(−3)	4.4(−2)	5.5(−3)	8.1(−3)	4.1(−4)	4.1(−2)
	10	3.6(−7)	7.5(−8)	3.7(−7)	5.6(−8)	3.9(−9)	4.2(−10)	3 7(−7)
	15	2.5(−9)	7.6(−8)	1.0(−8)	5.9(−8)	1.3(−10)	6.3(−10)	1.0(−10)
4.0	5	3.4(−1)	2.0(−1)	5.0(−1)	1.0(−1)	9.7(−2)	8.7(−3)	4.4(−1)
	10	1.3(−4)	6.1(−5)	2.7(−6)	2.0(−7)	1.4(−4)	4.2(−5)	1.3(−4)
	15	3.4(−9)	4.0(−8)	7.4(−9)	1.7(−8)	8.6(−10)	1.9(−10)	7.1(−10)
8.0	5	5.8(−1)	2.6(0)	2.4(0)	6.1(−1)	5.4(−1)	6.8(−2)	2.1(0)
	10	1.7(−2)	2.1(−2)	2.1(−2)	9.7(−3)	7.7(−4)	5.3(−5)	2.0(−2)
	15	5.8(−6)	1.4(−5)	6.3(−6)	8.4(−6)	1.3(−7)	1.2(−9)	6.1(−6)
	20	7.2(−7)	2.0(−7)	1.0(−8)	2.5(−7)	3.1(−10)	2.7(−10)	1.7(−9)

that the low order formulae of the finite difference method are superior to the corresponding Chebyshev formulae, but as the order increases the Chebyshev formulae become quickly more accurate for the same number of points. They have the added advantage of reasonable uniformity over the range of differentiation and the error can be estimated with some confidence in the manner shown. Both formulae exhibit rounding error effects if the order is increased beyond that which first yields machine accuracy where it will be observed that a maximum precision of only around 9 figures could be anticipated in each case using single precision (11 digit) arithmetic. This is seen in the $c = 0.5$ case of Table I where these results are carried out.

As a second more stringent test the routine was used on the function

$$\frac{1}{x} \sin \frac{1}{x}$$

with a varying interval so that the difficulty increased as the lower range of the interval approached the origin. The test intervals used were (1.0, 2.0), (0.5, 1.0) and (0.1, 0.5) and the results are tabulated in Table II. It is seen that the severe errors in the final range near the origin are adequately estimated. In fact the errors in this range are not as bad as they might appear from the actual absolute errors quoted, as the derivatives themselves are large. For instance at $x = 0.1$ the true derivative is 893.5 and the $M = 20$ formula predicts 894.8 whereas the finite difference formula yields 832.7. As percentage errors these are quite respectable for such a severe function.

TABLE II

Chebyshev and Lagrangian Absolute Errors for $f'(x)$ on $[A, B]$ where $f(x) = (1/x) \sin (1/x)$ with an $(M + 1)$ Point Formula

A	B	M	Actual Chebyshev error at A	Actual Lagrange error at A	Actual Chebyshev error at $(A + B)/2$	Actual Lagrange error at $(A + B)/2$	Estimated Error
1.0	2.0	5	1.2(−2)	6.8(−4)	2.4(−3)	1.1(−4)	1.3(−2)
		10	2.7(−5)	4.2(−5)	2.3(−6)	1.3(−7)	3.2(−5)
		15	3.0(−8)	1.1(−7)	4.2(−9)	6.3(−10)	3.5(−8)
		20	2.5(−8)	1.8(−6)	1.8(−9)	3.9(−10)	1.2(−9)
0.5	1.0	5	2.2(−1)	2.0(−1)	4.4(−2)	7.2(−3)	3.3(−1)
		10	3.4(−4)	1.2(−4)	2.9(−5)	7.6(−7)	3.5(−4)
		15	4.8(−7)	3.6(−6)	6.3(−9)	7.0(−10)	5.3(−7)
		20	1.5(−7)	3.8(−5)	3.2(−9)	7.0(−9)	1.2(−9)
0.1	0.5	5	1.2(1)	8.1(2)	9.9(1)	1.0(1)	3.1(2)
		10	1.6(2)	7.8(2)	1.2(1)	2.8(−1)	7.7(1)
		15	3.3(1)	2.3(2)	1.2(0)	1.1(−2)	2.8(1)
		20	1.3(0)	6.1(1)	6.5(−2)	9.1(−6)	2.5(0)

In conclusion therefore it appears that this is a practical proposition for numerical differentiation which is superior to the conventional finite difference approach in accuracy but has the added and important characteristic of yielding a reliable error estimate at any point.

REFERENCES

1. F. B. HILDEBRAND, "Introduction to Numerical Analysis," McGraw–Hill, New York, 1956.
2. J. C. SLATER, "Quantum Theory of Atomic Structure," McGraw–Hill, New York, 1960.
3. M. BLAKEMORE, G. A. EVANS, AND J. HYSLOP, *Int. J. Quantum Chem. XI* (1977), 325.
4. M. BLAKEMORE, G. A. EVANS, AND J. HYSLOP, *Int. J. Quantum Chem. XII* (1977), 305.
5. C. W. CLENSHAW AND A. R. CURTIS, *Numer. Math.* **2** (1960), 197.
6. C. C. J. ROOTHAAN, *Rev. Modern Phys.* **32** (1960), 179.
7. H. O'HARA AND F. H. SMITH, *Comput. J.* **11** (1968), 213.
8. D. R. HARTREE, *Rep. Progr. Phys.* **11** (1948), 113.

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