FORMULAE FOR NUMERICAL DIFFERENTIATION

By W G. Bickley.

In a recent paper (1) formulae were given for the numerical integration of a function in terms of its values at a set of arguments at equal intervals. In this companion paper, formulae for numerical differentiation, using the same data, are collected. Their utility in enabling derivatives of a function given numerically at such a set of arguments to be computed is obvious , the need arises in several approximate methods which are coming more and more into use (2), (3). The formulae avoid the labour of preliminary differencing, and are indeed more convenient than the finite difference formulae when the derivative is required at all the points of subdivision of a limited range.

Notation.

If $y=f(x)$ is a function of x, the value of y at $x_p=x_0+ph$ will be denoted by y_p ; h is the tabular interval, and p will (almost everywhere) denote an integer. With D denoting the differential operator, $D^m y_p$ will denote the mth derivative of y at x_p.

Basic formula and description of Tables (pp. 22-27).

The Tables give, for a set of values of the various parameters, the numerical values of ${}_{mn}A_{pr}$ and ${}_{mn}E_p$ in the formula

$$\frac{h^m D^m y_p}{m!}=\frac{1}{n!}\sum_{r=0}^{n} {}_{mn}A_{pr}y_r + {}_{mn}E_p.$$

(In the Tables, the suffixes m, n, and p are dropped, A_r and E simply being sufficient, since m, n, and p are explicitly given.) E is the "error" term, and is normally a multiple of $h^{n+1}D^{n+1}y(X)$, where X is some (unspecified) value of x between x_0 and x_n. Occasionally E is of a higher order , such cases are clearly indicated.

For $n=2(1)6$ the complete set of coefficients (*i.e.*, $p=0(1)n=m$) is given ; for $n=8$ and 10 advantage is taken of the symmetry of these matrices to save space. Also, in the latter cases, coefficients for the first four derivatives only are given ; if higher derivatives are required they may be obtained by repeated applications of the formula. For instance, D^6y can be computed by first finding $D^4y_p=z_p$ for $p=0(1)n$, and then computing D^2z_p.

Calculation and checking of coefficients.

It is clear that the A are multiples of the derivatives of the Lagrangian interpolation polynomials for the values x_p of x. For $n=2(1)6$ the coefficients were in fact calculated from these polynomials. For $n=7(1)10$ use was made of the formula

$${}_{mn}A_{pr}=n_{m,\,n-1}A_{pr}+(-)^{n-r}\binom{n}{r}{}_{mn}A_{pn}.$$

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The value of ${}_{mn}A_{pn}$ were obtained from tables prepared in connection with another investigation.

This formula was also used to check the coefficients for $n=2(1)6$. For $n=8$ and 10 (in calculating which the values for 7 and 9 had also to be obtained) the symmetry (or anti-symmetry) of the complete matrices was an almost conclusive check—after the few errors which it disclosed had been corrected, no further error was detected.

Finally, the proofs have been checked by means of the equations

$$\sum_{r=0}^{n} {}_{mn}A_{pr}=0, \quad \sum_{r=0}^{n} r\,{}_{mn}A_{pr}=\begin{matrix} n! \ (m=1) \\ 0 \ (m>1) \end{matrix},$$

which are the results of applying the formulae to the functions $y=1$ and $y=x$ with $h=1$.

The author wishes to thank Dr. J C. P Miller for an additional check.

A further application of the formulae.

The author's original idea as to the use of these formulae was their application to the step-by-step numerical integration of differential equations. Choosing n and h so that the error term is sufficiently small to justify the expectation that the desired degree of accuracy may be achieved, suppose that $y_0, y_1, \ldots y_{n-1}$ have been determined (*e.g.*, by Maclaurin's series). The successive derivatives of y at x_n are expressed in terms of $y_0, y_1, \ldots y_n$, and these expressions are substituted in the differential equation, which thereby becomes an algebraic equation for y_n.

Having thus determined y_n, we use $y_1, y_2, \ldots y_n$ to determine $y_{n+1} \ldots$, and so on.

The method is susceptible of elaboration and refinement, but we content ourselves here with a crude application to a very simple differential equation, namely to approximate to e^x as a solution of the equation $Dy=y$, taking $h=0{\cdot}1$.

By 3–1–3,

$$0{\cdot}1Dy_3=(11y_3-18y_2+9y_1-2y_0)/6$$

or, since $Dy_3=y_3$,

$$10{\cdot}4y_3=18y_2-9y_1+2y_0.$$

Similarly, $$10{\cdot}4y_4=18y_3-9y_2+2y_1,$$
and so on.

If we apply the more accurate formula 4–1–4, we find

$$47{\cdot}6y_4=96y_3-72y_2+32y_1-6y_0.$$

A start was made by use of the eight decimal values of e^x obtained from tables; they are given in column 1. Columns 2 and 3 give the results of successive applications of 3–1–3 and 4–1–4 respectively

	1	2	3
x	e^x	3–1–3	4–1–4
0·0	1·00000 000		
0·1	1·10517 092		
0·2	1·22140 276		
0·3	1·34985 881	1·34987 610	
0·4	1·49182 470	1·49187 373	1·49182 598
0·5	1·64872 127	1·64881 228	1·64872 527
0·6	1·82211 880	1·82226 054	1·82212 648
0·7	2·01375 271	2·01395 449	2·01376 473
0·8	2·22554 093	2·22581 352	2·22555 800
0·9	2·45960 311	2·45995 904	2·45962 612
1·0	2·71828 183	2·71873 558	2·71831 185

Enough decimals have been carried to ensure that the error is not obscured by " rounding-off errors " With 4–1–4, the error E at any stage is less than $10^{-5}y_n/5$—since $D^5y=y$—so that the sum of the errors due to the steps from y_4 to y_{10} is less than

$$\frac{1}{5}\times\frac{24}{47{\cdot}6}\times 10^{-5}\sum_4^{10} y_n = 1{\cdot}44\times 10^{-5}$$

The actual error at $x=1{\cdot}0$ turns out to be about double this,

$$(3{\cdot}0\ \ldots \times 10^{-5}).$$

The discrepancy is due, of course, to the cumulative effect of the errors of the approximation made in previous lines. It is possible to obtain a check which will indicate roughly the amount of the error at each stage, and so to correct it, and the elaborated and refined —but more laborious—procedure can be expected to give considerably reduced errors.

REFERENCES.

(1) W. G. Bickley, " Formulae for Numerical Integration ". *Math. Gazette*, XXIII, pp. 352-359, Oct. 1939.

(2) K. N. E. Bradfield and R. V. Southwell, " Relaxation Methods Applied to Engineering Problems ". *Proc. Roy. Soc.*, A, 161, pp. 155-181, July 1937.

(3) P. D. Crout, " An Application of Polynomial Approximation to the Solution of Integral Equations arising in Physical Problems ". *J. Math. and Phys.*, XIX, pp. 34-91, Jan. 1940. (Crout gives coefficients for $m=1$, 2, and 3, with $n=2$, 4, and 6.)

While stocks last, copies of this paper, and of the companion paper " Formulae for Numerical Integration " (*Math. Gazette*, XXIII, pp. 352-359, Oct. 1939), can be obtained from the author, Dr W G. Bickley, 27, Cuckoo Hill, Pinner, Middlesex, at a small charge to defray the cost of postage and off-prints, namely, 4d. per copy, or 4 copies for 1s., post free.

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n	m	p	A_0	A_1	A_2	A_3	E
2	1	0	−3	4	−1		+1/3 . $h^3 f^{iii}$
		1	−1	0	1		−1/6
		2	1	−4	3		+1/3
2	2	0	1	−2	1		−1/2
		1	1	−2	1		−1/24 . $h^4 f^{iv}$
		2	1	−2	1		+1/2 . $h^3 f^{iii}$
3	1	0	−11	18	−9	2	−1/4 $h^4 f^{iv}$
		1	−2	−3	6	−1	+1/12
		2	1	−6	3	2	−1/12
		3	−2	9	−18	11	+1/4
3	2	0	6	−15	12	−3	+11/24
		1	3	−6	3	0	−1/24
		2	0	3	−6	3	−1/24
		3	−3	12	−15	6	+11/24
3	3	0	−1	3	−3	1	−1/4
		1	−1	3	−3	1	−1/12
		2	−1	3	−3	1	+1/12
		3	−1	3	−3	1	+1/4

n	m	p	A_0	A_1	A_2	A_3	A_4	E
4	1	0	−50	96	−72	32	−6	+1/5 $h^5 f^{v}$
		1	−6	−20	36	−12	2	−1/20
		2	2	−16	0	16	−2	+1/30
		3	−2	12	−36	20	6	−1/20
		4	6	−32	72	−96	50	+1/5
4	2	0	35	−104	114	−56	11	−5/12
		1	11	−20	6	4	−1	+1/24
		2	−1	16	−30	16	−1	+1/180 . $h^6 f^{vi}$
		3	−1	4	6	−20	11	−1/24 . $h^5 f^{v}$
		4	11	−56	114	−104	35	+5/12
4	3	0	−10	36	−48	28	−6	+7/24
		1	−6	20	−24	12	−2	+1/24
		2	−2	4	0	−4	2	−1/24
		3	2	−12	24	−20	6	+1/24
		4	6	−28	48	−36	10	+7/24
4	4	0	1	−4	6	−4	1	−1/12
		1	1	−4	6	−4	1	−1/24
		2	1	−4	6	−4	1	−1/144 . $h^6 f^{vi}$
		3	1	−4	6	−4	1	+1/24 . $h^5 f^{v}$
		4	1	−4	6	−4	1	+1/12

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n	m	p	A_0	A_1	A_2	A_3	A_4	A_6	E
5	1	0	−274	600	−600	400	−150	24	$-1/6 . h^6 f^{vi}$
		1	−24	−130	240	−120	40	−6	+1/30
		2	6	−60	−40	120	−30	4	−1/60
		3	−4	30	−120	40	60	−6	+1/60
		4	6	−40	120	−240	130	24	−1/30
		5	−24	150	−400	600	−600	274	+1/6
5	2	0	225	−770	1070	−780	305	−50	+137/360
		1	50	−75	−20	70	−30	5	−13/360
		2	−5	80	−150	80	−5	0	+1/180
		3	0	−5	80	−150	80	−5	+1/180
		4	5	−30	70	−20	−75	50	−13/360
		5	−50	305	−780	1070	−770	225	+137/360
5	3	0	−85	355	−590	490	−205	35	−5/16
		1	−35	125	−170	110	−35	5	−1/48
		2	−5	−5	50	−70	35	−5	+1/48
		3	5	−35	70	−50	5	5	−1/48
		4	−5	35	−110	170	−125	35	+1/48
		5	−35	205	−490	590	−355	85	+5/16
5	4	0	15	−70	130	−120	55	−10	+17/144
		1	10	−45	80	−70	30	−5	+5/144
		2	5	−20	30	−20	5	0	−1/144
		3	0	5	−20	30	−20	5	−1/144
		4	−5	30	−70	80	−45	10	+5/144
		5	−10	55	−120	130	−70	15	+17/144
5	5	0	−1	5	−10	10	−5	1	−1/48
		1	−1	5	−10	10	−5	1	−1/80
		2	−1	5	−10	10	−5	1	−1/240
		3	−1	5	−10	10	−5	1	+1/240
		4	−1	5	−10	10	−5	1	+1/80
		5	−1	5	−10	10	−5	1	+1/48

n	m	p	A_0	A_1	A_2	A_3	A_4	A_5	A_6	E	
		0	−1764	4320	−5400	4800	−2700	864	−120	+1/7	. $h^7 f$ vii
		1	−120	−924	1800	−1200	600	−180	24	−1/42	
		2	24	−288	−420	960	−360	96	−12	+1/105	
6	1	3	−12	108	−540	0	540	−108	12	−1/140	
		4	12	−96	360	−960	420	288	−24	+1/105	
		5	−24	180	−600	1200	−1800	924	120	−1/42	
		6	120	−864	2700	−4800	5400	−4320	1764	+1/7	
		0	1624	−6264	10530	−10160	5940	−1944	274	−7/20	
		1	274	−294	−510	940	−570	186	−26	+11/360	
		2	−26	456	−840	400	30	−24	4	−1/180	
6	2	3	4	−54	540	−980	540	−54	4	−1/1120	$h^8 f$ viii
		4	4	−24	30	400	−840	456	−26	+1/180	$h^7 f$ vii
		5	−26	186	−570	940	−510	−294	274	−11/360	
		6	274	−1944	5940	−10160	10530	−6264	1624	+7/20	
		0	−735	3480	−6915	7440	−4605	1560	−225	+29/90	
		1	−225	840	−1245	960	−435	120	−15	+7/720	
		2	−15	−120	525	−720	435	−120	15	−1/90	
6	3	3	15	−120	195	0	−195	120	−15	+7/720	
		4	−15	120	−435	720	−525	120	15	−1/90	
		5	15	−120	435	−960	1245	−840	225	+7/720	
		6	225	−1560	4605	−7440	6915	−3480	735	+29/90	
		0	175	−930	2055	−2420	1605	−570	85	−7/48	
		1	85	−420	855	−920	555	−180	25	−1/36	
		2	25	−90	105	−20	−45	30	−5	+1/144	
6	4	3	−5	60	−195	280	−195	60	−5	+7/5760	$h^8 f$ viii
		4	−5	30	−45	−20	105	−90	25	−1/144	$h^7 f$ vii
		5	25	−180	555	−920	855	−420	85	+1/36	
		6	85	−570	1605	−2420	2055	−930	175	+7/48	
		0	−21	120	−285	360	−255	96	−15	+5/144	
		1	−15	84	−195	240	−165	60	−9	+1/72	
		2	−9	48	−105	120	−75	24	−3	+1/720	
6	5	3	−3	12	−15	0	15	−12	3	−1/360	
		4	3	−24	75	−120	105	−48	9	+1/720	
		5	9	−60	165	−240	195	−84	15	+1/72	
		6	15	−96	255	−360	285	−120	21	+5/144	
		0	1	−6	15	−20	15	−6	1	−1/240	
		1	1	−6	15	−20	15	−6	1	−1/360	
		2	1	−6	15	−20	15	−6	1	−1/720	
6	6	3	1	−6	15	−20	15	−6	1	−1/2880	$h^8 f$ viii
		4	1	−6	15	−20	15	−6	1	+1/720	$h^7 f$ vii
		5	1	−6	15	−20	15	−6	1	+1/360	
		6	1	−6	15	−20	15	−6	1	+1/240	

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n	m	p	A_0	A_1	A_2	A_3	A_4		E
8	1	0	−1 09584	3 22560	−5 64480	7 52640	−7 05600	8	+1/9 . $h^9 f^{\text{ix}}$
		1	−5040	−64224	1 41120	−1 41120	1 17600	7	−1/72
		2	720	−11520	−38304	80640	−50400	6	+1/252
		3	−240	2880	−20160	−18144	50400	5	−1/504
		4	144	−1536	8064	−32256	0	4	+1/630
		5	−144	1440	−6720	20160	−50400	3	−1/504
		6	240	−2304	10080	−26880	50400	2	+1/252
		7	−720	6720	−28224	70560	−1 17600	1	−1/72
		8	5040	−46080	1 88160	−4 51584	7 05600	0	+1/9
8	3	0	−67284	3 90880	−10 27768	16 06752	−16 31840	8	+29531/90720
		1	−13132	50904	−81872	75320	−47880	7	−1/5670
		2	−140	−11872	45864	−70112	57680	6	−331/90720
		3	252	−2408	−2800	24696	−38360	5	+59/22680
		4	−196	2016	−9464	13664	0	4	−41/18144
		5	196	−1960	9072	−25928	38360	3	+59/22680
		6	−252	2464	−11032	30240	−57680	2	−331/90720
		7	140	−1512	7504	−22792	47880	1	−1/5670
		8	13132	−1 18048	4 71240	−10 95584	16 31840	0	+29531/90720
			$-A_8$	$-A_7$	$-A_6$	$-A_5$	$-A_4$	p	

n	m	p	A_0	A_1	A_2	A_3	A_4		E
8	2	0	1 18124	−5 54112	12 51936	−17 94688	17 41320	8	−761/2520 $h^9 f^{\text{ix}}$
		1	13068	512	−83664	1 54224	−1 48120	7	+223/10080
		2	−1044	22464	−37072	4032	22680	6	−19/5040
		3	188	−2736	29232	−52864	27720	5	+1/1120
		4	−36	512	−4032	32256	−57400	4	+1/6300 $h^{10} f^{\text{x}}$
		5	−36	288	−784	−1008	27720	3	−1/1120 $h^9 f^{\text{ix}}$
		6	188	−1728	7056	−16576	22680	2	+19/5040
		7	−1044	9584	−39312	94752	−1 48120	1	−223/10080
		8	13068	−1 18656	4 80032	−11 37024	17 41320	0	+761/2520
8	4	0	22449	−1 47392	4 28092	−7 20384	7 69510	8	−89/480
		1	6769	−38472	96292	−1 40504	1 32510	7	−101/5760
		2	889	−1232	−6468	21616	−28490	6	+13/2880
		3	−231	2968	−9548	12936	−7490	5	−7/5760
		4	49	−672	4732	−13664	19110	4	−41/181440 . $h^{10} f^{\text{x}}$
		5	49	−392	1092	616	−7490	3	+7/5760 . $h^9 f^{\text{ix}}$
		6	−231	2128	−8708	20496	−28490	2	−13/2880
		7	889	−8232	34132	−83384	1 32510	1	+101/5760
		8	6769	−60032	2 35452	−5 34464	7 69510	0	+89/480
			A_8	A_7	A_6	A_5	A_4	p	

n	m	p	A_0	A_1	A_2	A_3	A_4	A_5		E
		0	−106 28640	362 88000	−816 48000	1451 52000	−1905 12000	1828 91520	10	+1/11 . $h^{11} f^{xi}$
		1	−3 62880	−66 36960	163 29600	−217 72800	254 01600	−228 61440	9	−1/110
		2	40320	−8 06400	−44 19360	96 76800	−84 67200	67 73760	8	+1/495
		3	−10080	1 51200	−13 60800	−27 56160	63 50400	−38 10240	7	−1/1320
		4	4320	−57600	3 88800	−20 73600	−13 30560	43 54560	6	+1/2310
10	1	5	−2880	36000	−2 16000	8 64000	−30 24000	0	5	−1/2772
		6	2880	−34560	1 94400	−6 91200	18 14400	−43 54560	4	+1/2310
		7	−4320	50400	−2 72160	9 07200	−21 16800	38 10240	3	−1/1320
		8	10080	−1 15200	6 04800	−19 35360	42 33600	−67 73760	2	+1/495
		9	−40320	4 53600	−23 32800	72 57600	−152 40960	228 61440	1	−1/110
		10	3 62880	−40 32000	204 12000	−622 08000	1270 08000	−1828 91520	0	+1/11
		0	−84 09500	575 37360	−1877 95260	3845 55840	−5419 68840	5429 59200	10	+16103/50400
		1	−11 72700	44 90200	−69 61140	57 00240	−24 35160	−1 81440	9	−41/11200
		2	8540	−12 66640	49 59900	−83 70240	85 18440	−63 80640	8	−593/453600
		3	7900	−78360	−8 32140	36 56400	−57 63240	48 68640	7	+263/302400
		4	−5340	66640	−3 72060	48960	18 94200	−32 96160	6	−13/21600
10	3	5	4100	−50440	2 92140	−10 48560	14 01960	0	5	+479/907200
		6	−4100	49200	−2 75940	9 68640	−24 01560	32 96160	4	−13/21600
		7	5340	−62840	3 42900	−11 57040	27 30840	−48 68640	3	+263/302400
		8	−7900	92240	−4 97340	16 46400	−37 64040	63 80640	2	−593/453600
		9	−8540	86040	−3 77460	9 11760	−11 71800	1 81440	1	−41/11200
		10	11 72700	−129 08240	645 84540	−1938 72960	3879 02760	−5429 59200	0	+16103/50400
			$-A_{10}$	$-A_9$	$-A_8$	$-A_7$	$-A_6$	$-A_5$	p	

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n	m	p	A_0	A_1	A_2	A_3	A_4	A_5		E	
		0	127 53576	−699 98400	1983 20400	−3767 61600	5103 75600	−4991 05152	10	−671/2520	$. h^{11} f^{xi}$
		1	10 26576	14 61240	−135 36720	289 35360	−379 91520	360 97488	9	+419/25200	
		2	−69264	17 88480	−23 48280	−21 08160	60 78240	−59 91552	8	−31/12600	
		3	11016	−1 90440	23 94360	−41 65920	15 27120	9 88848	7	+29/50400	
		4	−2664	40320	−3 36960	28 33920	−50 45040	27 57888	6	−1/6300	
10	2	5	576	−9000	72000	−4 32000	30 24000	−53 11152	5	−1/33264	$h^{12} f^{xii}$
		6	576	−5760	22680	−23040	−2 41920	27 57888	4	+1/6300	$h^{11} f^{xi}$
		7	−2664	29880	−1 52280	4 62240	−9 02160	9 88848	3	−29/50400	
		8	11016	−1 23840	6 35760	−19 69920	40 97520	−59 91552	2	+31/12600	
		9	−69264	7 72920	−39 33360	120 64320	−248 27040	360 97488	1	−419/25200	
		10	10 26576	−113 61600	572 34600	−1733 18400	3508 34400	−4991 05152	0	+671/2520	
		0	34 16930	−265 57640	953 16120	−2081 94720	3060 06540	−3152 46960	10	−7645/36288	$h^{11} f^{xi}$
		1	7 23680	−45 43550	132 44760	−240 91080	306 19680	−283 33620	9	−2041/181440	
		2	50840	1 64440	−17 47350	48 56160	−73 13880	71 31600	8	+167/60480	
		3	−12790	1 91530	−5 39010	3 63000	6 35460	−14 04900	7	−277/362880	
		4	3590	−52280	3 88980	−11 31360	15 47700	−10 23120	6	+41/181440	
10	4	5	−820	12610	−97380	5 24280	−14 01960	19 26540	5	+479/10886400	$h^{12} f^{xii}$
		6	−820	8200	−32490	37920	2 53680	−10 23120	4	−41/181440	$h^{11} f^{xi}$
		7	3590	−40310	2 05650	−6 24840	12 22620	−14 04900	3	+277/362880	
		8	−12790	1 44280	−7 43760	23 16000	−48 45540	71 31600	2	−167/60480	
		9	50840	−5 72030	29 40480	−91 32360	190 93200	−283 33620	1	+2041/181440	
		10	7 23680	−79 09640	392 30370	−1164 66720	2296 82040	−3152 46960	0	+7645/36288	
			A_{10}	A_9	A_8	A_7	A_4	A_5	p		

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