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Step-by-Step Integration of $\ddot{x} = f(x, y, z, t)$ without a "Corrector"

Introduction.—For step-by-step numerical integration of ordinary differential equations there are too many formulae, too few evaluations or comparisons. Perhaps the complexity of the subject will not permit the generalizations the mathematician would prefer, but only restricted numerical comparisons of specific procedures. This paper, at any rate, will restrict itself to showing reasons for preferring one of two procedures for the integration of second-order differential equations in which the second derivative, $\ddot{x} = \dfrac{d^2x}{dt^2}$, is a function of x alone, or of x and t, or of x, y, z, t (with similar equations for $\ddot{y}$ and $\ddot{z}$). These equations are important, of course, in certain dynamical problems of astronomy, ballistics, aerodynamics, etc., including the rocket problem.

The comparison of the two procedures will extend to at least three equivalent forms, in which the integration formula at each step is based upon

(a) antecedent values of $\ddot{x}$,
(b) backwards differences of $\ddot{x}$,
(c) central differences (estimated) of $\ddot{x}$.

Although there are reasons for preferring forms (a) or (b) in certain circumstances, the comparison will be made first between the procedures in form (c) because there is some advantage to distinguishing between errors of estimation and errors resulting from the neglect of higher order terms in the integration formulae.

The preferred procedure, designated the "second-sum procedure" or "Σ^2 procedure," involves tables of $\ddot{x}$ and its first and second sums, $\Sigma\ddot{x}$ and $\Sigma^2\ddot{x}$, as well as its differences (explicitly or implicitly), $\delta\ddot{x}$, $\delta^2\ddot{x}$, $\delta^3\ddot{x}$, $\cdots$. It has been used for more than a century by astronomers,[1,2] but has apparently been overlooked by a number of mathematicians, physicists, and others, in recent years.

The compared procedure, designated the "second-difference procedure" or "δ^2 procedure," involves the summation (explicit or implicit) of the second difference of x, δ^2x, which is obtained by formula from $\ddot{x}$ and its differences (or the equivalent). This procedure was used by COWELL & CROMMELIN, perhaps for the first time in an extended calculation, in their celebrated prediction of the return of Halley's Comet in 1910. In publishing the results of this work[3] they recommended without explanation, however, that future integrations of this type should be done with the Σ^2 procedure and formulae. In spite of this recommendation a great deal of work has been done by the

δ^2 procedure, by astronomers as well as others, that could have been shown to be better adapted to the Σ^2 procedure.

In short this paper will show that (1) under comparable circumstances, the δ^2 procedure requires two approximations (or the use of "predictor" and "corrector" formulae[8]) whereas the Σ^2 procedure requires only one. It will show further that (2) the estimated differences normally employed by the astronomer may be replaced by backwards differences or antecedent values of the second difference without increasing the error or requiring a second approximation. The second of these facts, as well as the first, is significant to modern calculation with automatic electronic digital computers.

The δ^2 Procedure.—For the purposes of the comparison it will be necessary first to outline the "δ^2 procedure" with estimated central differences, since these may be unfamiliar to many persons otherwise well acquainted with the problem. Their introduction makes it possible to use the same formula for "predictor" and "corrector," the difference between the two approximations being due to the improvement in the estimates of the differences involved. This formula[7] we shall call the "(δ_c^2) formula" and write as follows:

$$(\delta_c^2) \qquad \delta^2 x_n = h^2 \left\{ \ddot{x}_n + \frac{1}{12}\,\delta^2\ddot{x}_n - \frac{1}{240}\,\delta^4\ddot{x}_n + \frac{31}{60480}\,\delta^6\ddot{x}_n - \cdots \right\}$$

where h is the interval of the argument (0.1 in the table below), the notation for the differences is best appreciated by reference to the numerical table below, and the subscript n indicates that the various quantities are to be found on the same line of the table (the underlined quantities on the 0.8 line in the example below).

The following table shows an integration table for the simple differential equation $\ddot{x} = -x$. How the table was started is not significant; at the given step all numbers not in parentheses may be taken as correct. The values of the differences of $\ddot{x}$ in parentheses are estimates based upon the assumption that the sixth difference is zero. The estimates of $\delta^2 x_{0.8}$, $\delta x_{0.85}$, and $x_{0.9}$, on the other hand, are a result of the first approximation or "prediction" below the table.

t	x	δx	$\delta^2 x$	$\ddot{x} = -x$	$\delta\ddot{x}$	$\delta^2\ddot{x}$	$\delta^3\ddot{x}$	$\delta^4\ddot{x}$	$\delta^5\ddot{x}$
0.0	+.000 000 000		000 000	−.000 0000		0000		000	
		+99 833 417			−99 8334		+9975		−100
0.1	+.099 833 417		−997 502	−.099 8334		+9975		−100	
		+98 835 915			−98 8359		+9875		−97
0.2	+.198 669 332		−1985 038	−.198 6693		+19850		−197	
		+96 850 877			−96 8509		+9678		−100
0.3	+.295 520 209		−2952 740	−.295 5202		+29528		−297	
		+93 898 137			−93 8981		+9381		−91
0.4	+.389 418 346		−3890 939	−.389 4183		+38909		−388	
		+90 007 198			−90 0072		+8993		−89
0.5	+.479 425 544		−4790 261	−.479 4255		+47902		−477	
		+85 216 937			−85 2170		+8516		−89
0.6	+.564 642 481		−5641 721	−.564 6425		+56418		−566	
		+79 575 216			−79 5752		+7950		(−89)
0.7	+.644 217 697		−6436 810	−.644 2177		+64368		(−655)	
		+73 138 406			−73 1384		(+7295)		(−89)
0.8	+.717 356 103		$\underline{(-7167\ 586)}$	$\underline{-.717\ 3561}$		$\underline{(+71663)}$		$\underline{(-744)}$	
		(+65 970 820)							
0.9	(+.783 326 923)								

	"Prediction"	"Correction"
$+\quad \ddot{x}_{0.8} =$	$-0.717\ 3561$	$-0.717\ 3561$
$+\ \frac{1}{12}\delta^2\ddot{x}_{0.8} =$	$+5971\ .9$	$+5973\ .0$
$-\ \frac{1}{240}\delta^4\ddot{x}_{0.8} =$	$\underline{+3\ .1}$	$\underline{+3\ .0}$
$h^{-2}\delta^2x_{0.8} =$	$-0.716\ 7586\ .0$	$-0.716\ 7585\ .0$
$\delta^2x_{0.8} =$	$-.007167586$	$-.007167585$

After the predicted $\delta^2x_{0.8}$ is summed in the table to produce an estimate of $x_{0.9}$, it is possible to calculate accurately $\ddot{x}_{0.9} = -0.783\ 3269$. [From an inspection of the "correction" we may verify that no significant revision of this number will be necessary.] The table may now be differenced to show that the accurate value of $\delta^2\ddot{x}_{0.8} = +71676$, and this number replaces the estimate ($+71663$) in the "correction," with a resulting change of one digit in $\delta^2x_{0.8}$, $\delta x_{0.85}$, and $x_{0.9}$. The table is now ready for the next step.

The Σ^2 Procedure.—The "(Σ_c^2) formula" is as follows:

$$(\Sigma_c^2) \qquad x_n = h^2\left\{\Sigma^2\ddot{x}_n + \frac{1}{12}\ddot{x}_n - \frac{1}{240}\delta^2\ddot{x}_n + \frac{31}{60480}\delta^4\ddot{x}_n - \cdots\right\}$$

where the notation is the same as in the (δ_c^2) formula. The numerical coefficients are the same in the two formulae because the one is simply the second sum or the second difference of the other. The table associated in this procedure with the numerical example of the preceding section is as follows:

t	$\Sigma^2\ddot{x}$	$\Sigma\ddot{x}$	$\ddot{x} = -x$	$\delta\ddot{x}$	$\delta^2\ddot{x}$	$\delta^3\ddot{x}$	$\delta^4\ddot{x}$	$\delta^5\ddot{x}$
0.0	+0.000 0000		−.000 0000		0000		000	
		+9.991 6653		−99 8334		+9975		−100
0.1	+9.991 6653		−.099 8334		+9975		−100	
		+9.891 8319		−98 8359		+9875		−97
0.2	+19.883 4972		−.198 6693		+19850		−197	
		+9.693 1626		−96 8509		+9678		−100
0.3	+29.576 6598		−.295 5202		+29528		−297	
		+9.397 6424		−93 8981		+9381		−91
0.4	+38.974 3022		−.389 4183		+38909		−388	
		+9.008 2241		−90 0072		+8993		−89
0.5	+47.982 5263		−.479 4255		+47902		−477	
		+8.528 7986		−85 2170		+8516		−89
0.6	+56.511 3249		−.564 6425		+56418		−566	
		+7.964 1561		−79 5752		+7950		(0)
0.7	+64.475 4810		−.644 2177		+64368		(−566)	
		+7.319 9384		−73 1384		(+7384)		(0)
0.8	+71.795 4194		−.717 3561		(+71752)		(−566)	
		+6.602 5823		(−65 9632)		(+6818)		
0.9	+78.398 0017		(−.783 3193)		(+78570)			

NOTE 1: The estimates of the differences (in parentheses) are arbitrarily made poorer in this example than in that of the preceding section, to emphasize the fact that an even larger error of estimation will not require a second approximation in the Σ^2 procedure.

NOTE 2: (For those unfamiliar with sum columns.) Given a starting value, the numbers in the $\Sigma\ddot{x}$ column are summed from the $\ddot{x}$ column just as the $\ddot{x}$ column could be summed from the $\delta\ddot{x}$ column. Similarly the $\Sigma^2\ddot{x}$ column is summed from the $\Sigma\ddot{x}$ column. Starting values may be obtained by an inversion of the process followed below.

NOTE 3: The subscript n refers to the 0.9 line in this example rather than the 0.8 line, as indicated by the underlining, in order to make the figures of the two examples more directly comparable.

The calculation of $x_{0.9}$ and of an accurate value of $\ddot{x}_{0.9}$ to replace the estimate of this quantity proceeds as follows, in accordance with equation (Σ_c^2):

$$
\begin{array}{rrl}
+ & \Sigma^2\ddot{x}_{0.9} = & +\ 78.398\ \ 00\ \ 2 \\
+\dfrac{1}{12} & \ddot{x}_{0.9} = & \qquad -65\ \ 27\ \ 7 \\
-\dfrac{1}{240} & \delta^2\ddot{x}_{0.9} = & \qquad\quad -3\ \ 3 \\
\hline
 & h^{-2}\,x_{0.9} = & +\ 78.332\ \ 69\ \ 2 \\
\ddot{x}_{0.9} = & -x_{0.9} = & -\ \ 0.783\ 3269
\end{array}
$$

Although this value of $\ddot{x}_{0.9}$ differs by 76 units of the last place from the estimate in the table, it will be found, in checking the figures of a possible "correction" or recalculation, that the preliminary value of $\frac{1}{12}\ddot{x}_{0.9}$, and hence the final value of $\ddot{x}_{0.9}$, will not be altered from what is shown in the above calculation. Nor would they if an even greater error were made in the estimate.

Comparison.—1. It will be observed, in the numerical work of the two examples, that the $\frac{1}{12}$ term involves in the first a 5 digit number ($\delta^2\ddot{x}_{0.8} = +71663$), in the second a 7 digit number ($\ddot{x}_{0.9} = -7833193$), but that only 5 digits are carried in either calculation ($+59719$ and -65277). That is in the Σ^2 procedure the last two digits of the estimate of $\ddot{x}$ are of no significance, and a much larger estimation error can be tolerated than in the $\delta^2\ddot{x}$ that plays the same role in the δ^2 procedure. Thus the first approximation is sufficient in the Σ^2 procedure, but a second is necessary in the δ^2 procedure to alter or check the last digit in the calculation. It is assumed, it will be noted, that successive columns of sums, function, and differences taper off in size by about one digit or more per column. When the tapering is more, the situation is even more favorable to the Σ^2 procedure: for example, if there are four more digits in the $\Sigma^2\ddot{x}$ column than in the $\ddot{x}$ column, the last four digits of the estimate of $\ddot{x}$ will not be significant, and a very crude estimate is tolerable. A tapering of one digit per column is probably the least that would be tolerated in any procedure for numerical integration when automatic or rote methods are employed; an experienced computer, using the utmost of judgment, may be able to integrate by these procedures when the tapering is only one digit per two columns.

2. Since a larger estimation error can be tolerated in the Σ^2 procedure than in the δ^2 procedure, it is evident that fewer difference columns will need to be taken into account, an advantage when the memory of an automatic computer is limited.

3. It is assumed that the accumulation of rounding error and the effect of neglected terms will be about the same in the two procedures. The discussion is concerned instead with the effect of errors of estimation, explicitly as in the foregoing example or implicitly in equivalent processes involving backwards differences or antecedent values of $\ddot{x}$. (The estimation of differences should not be confused with a first approximation or "prediction," but should be recognized as merely an alternative way of making the integration depend upon backwards differences.)

4. It is assumed that the purpose of numerical integration is the construction of as accurate as possible a table from which the integral may be obtained, and not necessarily a table of the integral itself. Often, as in comet orbits or ballistics tables, only a few values of the integral at the end of the table are needed. Since, however, it is customary to carry two or three more places in a table than are required in the end, it will be noted that the values of the integral obtained in the first approximation by either procedure are probably sufficiently accurate for all intended uses. From this point of view, evidently the second approximation in the δ^2 procedure is necessary only to avoid the accumulation of error in the summation of $\delta^2 x$. The equivalent summation of $\ddot{x}$ in the Σ^2 procedure is free of estimation error. For interpolating non-tabular values of the integral, BOWER has supplied a table.[6]

5. To shorten the paper, I have not included in the foregoing discussion a third procedure which may be used in integration of second-order differential equations. This procedure is based upon the formula for the second derivative, $\ddot{x}$, in terms of the differences of x, which we may write

$$\delta^2 x = h^2\ddot{x} + \frac{1}{12}\,\delta^4 x - \frac{1}{90}\,\delta^6 x + \cdots.$$

My investigation of this procedure revealed only a greater disadvantage: namely, three approximations as compared with the two of the δ^2 procedure and the one of the Σ^2 procedure. Various attempts have been made to improve this formula for restricted classes of second-order differential equations by introducing special devices to eliminate the $\frac{1}{12}$ term—beginning with NUMEROV,[4] and most recently by FOX & GOODWIN.[9] At best these devices yield results comparable to the Σ^2 procedure only when the $1/240$ term is negligible, and at least for some of them JACKSON[5] is right in believing that they would become the Σ^2 procedure if they were carried to their logical conclusion.

Another proposal sometimes made in connection with the second-derivative formula above is that it be used to correct a first approximation in which the estimation error is ignored. This proposal would have merit if it were not for the fact that the estimation error is negligible in the first approximation by the Σ^2 procedure.

The Backwards-Difference Formula.—When the central differences used in the $(\Sigma_c{}^2)$ formula are estimated by a summation based upon the repetition of the last value of a given difference, the calculation will yield exactly the same result as if it had been based upon a backwards-difference formula ending with the same difference. This formula is as follows:

$$(\Sigma_b{}^2) \qquad x_n = h^2\left\{\Sigma^2\ddot{x}_n + \frac{1}{12}\left[\ddot{x}_{n-1} + \delta\ddot{x}_{n-3/2} + \frac{19}{20}\,\delta^2\ddot{x}_{n-2} + \frac{18}{20}\,\delta^3\ddot{x}_{n-5/2} + \frac{1726}{2016}\,\delta^4\ddot{x}_{n-3} + \frac{1650}{2016}\,\delta^5\ddot{x}_{n-7/2} + \cdots\right]\right\}.$$

The estimation of differences may thus be entirely avoided in rote calculation, by automatic machinery or otherwise.

The Antecedent-Function Formula.—When the computer feels that he can dispense with the check afforded by the run of the differences, he may replace the (Σ_b^2) formula by the equivalent expression in terms of antecedent values of the function to be integrated:

$$(\Sigma_a^2) \qquad x_n = h^2 \left\{ \Sigma^2 \ddot{x}_n + \frac{1}{12}\left(1 + 1 + \frac{19}{20} + \frac{18}{20} + \cdots\right) \ddot{x}_{n-1} - \frac{1}{12}\left(1 + 2\cdot\frac{19}{20} + 3\cdot\frac{18}{20} + \cdots\right) \ddot{x}_{n-2} + \frac{1}{12}\left(\frac{19}{20} + 3\cdot\frac{18}{20} + \cdots\right) \ddot{x}_{n-3} - \frac{1}{12}\left(\frac{18}{20} + \cdots\right) \ddot{x}_{n-4} + \cdots \right\}.$$

It is evident that this general expression will yield a number of formulae, depending upon the order of the last difference of the (Σ_b^2) formula that is taken into account:

$$(\Sigma_a^2)_0 \qquad x_n = h^2 \left\{ \Sigma^2 \ddot{x}_n + \frac{1}{12} \ddot{x}_{n-1} \right\}$$

$$(\Sigma_a^2)_1 \qquad x_n = h^2 \left\{ \Sigma^2 \ddot{x}_n + \frac{1}{12} (2\ddot{x}_{n-1} - \ddot{x}_{n-2}) \right\}$$

$$(\Sigma_a^2)_2 \qquad x_n = h^2 \left\{ \Sigma^2 \ddot{x}_n + \frac{1}{240} (59\ddot{x}_{n-1} - 58\ddot{x}_{n-2} + 19\ddot{x}_{n-3}) \right\}$$

$$(\Sigma_a^2)_3 \qquad x_n = h^2 \left\{ \Sigma^2 \ddot{x}_n + \frac{1}{240} (77\ddot{x}_{n-1} - 112\ddot{x}_{n-2} + 73\ddot{x}_{n-3} - 18\ddot{x}_{n-4}) \right\}$$

and so on, where $(\Sigma_a^2)_m$ includes the effect of $\delta^m \ddot{x}$.

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Formulas for Calculating the Error Function of a Complex Variable

1. Various methods have been suggested for the computation, to high accuracy, of the error function $\Phi(Z) = \int_0^Z e^{-u^2} du$ for complex arguments $Z = X + iY$. The Maclaurin series is convenient for extreme accuracy only when $|Z|$ is small, and the asymptotic expansions[1] are useful only for fairly large values of $|Z|$. Other less elementary methods (e.g., the AIREY converging factor,[2] or the continued fraction expansion[1]) have limited success in certain regions of the Z-plane. The most convenient methods for calculating $\Phi(Z)$ to very many figures are described in the works of MILLER & GORDON[3] and ROSSER.[4] It is the purpose of this note, which is self-contained, to present in a concise and practical form, two schemes for the computation of $\Phi(Z)$ which follow the main ideas of Miller, Gordon, and Rosser.

2. The basis of the present methods is the following formula:

$$(1) \qquad \sum_{n=-\infty}^{\infty} \exp\left(-(u + na)^2\right) = \pi^{\frac{1}{2}} a^{-1} \sum_{n=-\infty}^{\infty} \exp\left(-n^2\pi^2 a^{-2}\right) \cos\left(2n\pi u/a\right)$$

which is an immediate corollary of POISSON's formula.[5] Formula (1) is also essentially Jacobi's imaginary transformation,[6] which has long been familiar to a number of mathematicians and physicists.[7,8] Also, (1) was used by DAWSON[9] in his computation of $\int_0^Y e^{u^2} du$. Two different methods for calculating $\Phi(Z)$ are given here in **4** and **5**. In all formulas, summations are from 1 to ∞ except where otherwise noted. The symbol $\doteq$ will denote approximate equality.

3. Dawson's formula for $\int_0^Y e^{u^2} du$ is needed in the second method. It follows from the approximate equality obtained from (1), which is

$$(2) \qquad e^{u^2}(1 + E) = a\pi^{-\frac{1}{2}}\left(1 + 2 \sum \exp\left(-a^2 n^2\right) \cosh 2nau\right), \qquad a \leqslant 1$$

where the relative error $E = 2 \sum e^{-n^2\pi^2/a^2} \cos\left(2n\pi u/a\right)$, is of the order of magnitude of $2e^{-\pi^2/a^2}$, since $2e^{-4\pi^2/a^2}$ is very small by comparison. Approximate values of E are given in the following table:

a	1	0.9	0.8	0.7	0.6	0.5
E	10^{-4}	10^{-5}	$\frac{1}{2}\cdot 10^{-6}$	$\frac{1}{2}\cdot 10^{-8}$	$\frac{1}{4}\cdot 10^{-11}$	$\frac{3}{2}\cdot 10^{-17}$

Putting $a = \frac{1}{2}$ in (2) Dawson obtains

$$(3) \qquad e^{u^2} \doteq \pi^{-\frac{1}{2}}\left(\tfrac{1}{2} + \sum e^{-n^2/4} \cosh nu\right),$$

the relative error in (3) being less than $2 \cdot 10^{-17}$. Then integration of (3) results in

$$(4) \qquad \int_0^Y e^{u^2} du \doteq \pi^{-\frac{1}{2}}\left(\tfrac{1}{2} Y + \sum n^{-1} \exp\left(-n^2/4\right) \sinh nY\right).$$