A Method for the Numerical Integration of Differential Equations of Second Order Without Explicit First Derivatives [1]

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This is a fourth-order step-by-step method based on difference formulas. The case of a single equation is discussed in detail. The use of this method for automatic computer is considered.

1. Introduction

This is a fourth-order step-by-step method based on difference formulas. The start of the computation is easy. Only the case of a single differential equation

$$\frac{d^2y}{dx^2} = f(x,y) \tag{1}$$

will be considered. The generalization to a set of differential equations

$$\frac{d^2y_i}{dx^2} = f_i(x,y_k) \qquad i,k = 1,2,\ldots,n$$

is immediate. Application to electronic computing is discussed.

2. General Formulas

We first note some general formulas that may be deduced, for instance, from the expressions (1.32), (1.38), (1.39), and (4.15) of L. Collatz [1]:[3]

$$\int_0^x \int_0^x f(x)dx^2 = {}^{(2)}f(x) - {}^{(2)}f(0) - {}^{(1)}f(0)x$$
$$= h^2 \sum_{p=0} P_{2,p}(u)\Delta^p f_{-p} \tag{2}$$
$$= h^2 \sum_{p=0} (-1)^p P_{2,p}(-u)\Delta^p f_0 \tag{3}$$

where $x = uh$,

$$P_{2,0}(u) = u^2/2; \quad P_{2,1}(u) = u^3/6; \quad P_{2,2}(u) = (2u^3 + u^4)/24; \quad P_{2,3}(u) = (20u^3 + 15u^4 + 3u^5)/360; \quad \ldots \tag{4}$$

and

$$^{(n)}f = \int_a^x {}^{(n-1)}f dx \qquad {}^{(0)}f = f, \quad n = 1,2.$$

Finally,

$$^{(1)}f_2 - {}^{(1)}f_0 = h(2f_1 + \frac{1}{3}\Delta^2 f_0 - \frac{1}{90}\Delta^4 f_{-1} + \ldots). \tag{5}$$

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[3] Figures in brackets indicate the literature references at the end of this paper.

The degree of approximation of the formulas given below is written in terms of the interval h; the symbol $\{n\}$ is equivalent to the usual $o(h^n)$. The following remarks are needed:

(1) f, computed from its definition, is of the same order of approximation as that of the y used;

(2) if $\Delta^{p+1}f$ is neglected in (2) or (3), these expressions are correct to the $(p+2)$nd order;

(3) if $\Delta^4 f_{-1}$ is neglected in (5), this formula is correct to the fourth order. In the notation introduced, the differential equation under consideration can be written as

$$y = {}^{(2)}f;$$

we shall also write

$$\frac{dy}{dx} = {}^{(1)}f = z.$$

3. Particular Formulas

When $x=h$, and if $\Delta^2 f_{-2}$ is neglected, (2) becomes

$$y_1 = y_0 + hz_0 + h^2(-f_{-1} + 4f_0)/6, \qquad \{3\} \tag{6}$$

provided $y_0\{3\}$, $z_0\{2\}$, and $f_0\{1\}$, $f_{-1}\{1\}$.

If Δf_{-1} is neglected in the same formula (2), we have

$$\tilde{y}_1 = y_0 + hz_0 + h^2 f_0/2. \qquad \{2\} \tag{7}$$

When $x=h$, and if $\Delta^2 f_0$ is neglected, (3) becomes

$$y_1 = y_0 + hz_0 + h^2(2f_0 + f_1)/6, \qquad \{3\} \tag{8}$$

provided $y_0\{3\}$, $z_0\{2\}$, and $f_0\{1\}$, $f_1\{1\}$.

The same formula yields, for $x=2h$, and with $\Delta^3 f_0$ neglected, since $P_{2,2}(-2)=0$,

$$y_2 = y_0 + 2hz_0 + h^2(2f_0 + 4f_1 + 0f_2)/3, \qquad \{4\} \tag{9}$$

and provided $y_0\{4\}$, $z_0\{3\}$, and $f_0\{2\}$, $f_1\{2\}$.

Neglecting $\Delta^4 f_{-1}$, (5) gives the Simpson formula

$$z_2 = z_0 + h(f_0 + 4f_1 + f_2)/3 \qquad \{4\} \tag{10}$$

if $z_0\{4\}$ and $f_0\{3\}$, $f_1\{3\}$, $f_2\{3\}$.

Finally, when $x=2ht$, and if $\Delta^3 f_0$ is neglected, (3) becomes

$$y = y_0 + 2hz_0 t + 2h^2 f_0 t^2 + \tfrac{2}{3}h^2(-3f_0 + 4f_1 - f_2)t^3 + \tfrac{2}{3}h^2(f_0 - 2f_1 + f_2)t^4. \qquad \{4\} \tag{11}$$

4. Integration Method

We are now ready to explain our method for solving differential equations of second order that do not contain the first derivatives explicitly. The starting value of the independent variable will be taken as zero. Each step is subdivided into two intervals of length h.

The general step will be considered first. Therefore, we will suppose that $f=f_{-1}\{3\}$ is known for $x=(2n-1)h$, and that $y=y_0\{4\}$, $f=f_0\{4\}$, $z=z_0\{4\}$, are known for $x=2nh$.

Then for $x=(2n+1)h$, $y=y_1\{3\}$ is given by (6) and $f=f_1\{3\}$ is given by (1), whereas for $x=(2n+2)h$, $y=y_2\{4\}$ is given by (9), $f=f_2\{4\}$ by (1) and $z=z_2\{4\}$ by (10).

These values will then serve for the next step. The process is of fourth order for the function as well as for its first derivative.

Two equivalent methods may be used to compute the first step. For $x=0$, and with initial conditions $y=y_0$ and $z=z_0$, $f=f_0$ is computed by means of the differential equation.

Then

(a). A preliminary calculation may be done with (7) and (1) so as to give

$$y=\tilde{y}_1\{2\} \text{ and } f=\tilde{f}_1\{2\}, \text{ for } x=h.$$

Then formula (8) may be used with $f_1=\tilde{f}_1$; this gives

$$y=y_1\{3\} \text{ and } f=f_1\{3\}, \text{ for } x=h.$$

The computation of the values for $x=2h$ is the same as for the general step $(2n+2)h$.

(b). Or, alternatively, it is also possible first to go backwards with the formula equivalent to (7),

$$y_{-1}=y_0-hz_0+h^2f_0/2. \quad \{2\}$$

The process for the general step may then be used for $x=h$ and $x=2h$ because (6) requires only a knowledge of f_{-1} to the first order and this function is known to the second.

Table 1 gives the coefficients of the z and f functions, (the coefficient of y is always one) for certain intervals between 0.50 and 0.06; if the interval to be chosen is outside this range, it is preferable, especially with the use of desk machines, to change the independent variable; this will prevent rounding off errors or the need of computation with an excess of decimal places.

TABLE 1.

For the users' convenience, certain entries have been repeated.

Intervals	Coefficients in formulas—													
	(6)			(9)			(10)	(7)		(8)			(7)	
	z_0	$-f_{-1}$	f_0	z_0	f_0	f_1	$f_0+4f_1+f_2$	z_0	f_0	z_0	f_0	f_1	$-z_0$	f_0
h	h	$h^2/6$	$2h^2/3$	$2h$	$2h^2/3$	$4h^2/3$	$h/3$	h	$h^2/2$	h	$h^2/3$	$h^2/6$	h	$h^2/2$
0.060000	0.060000	0.000600	0.002400	0.120000	0.002400	0.004800	0.020000	0.060000	0.001800	0.060000	0.001200	0.000600	0.060000	0.001800
.075000	.075000	.000938	.003750	.150000	.003750	.007500	.025000	.075000	.002813	.075000	.001875	.000938	.075000	.002813
.090000	.090000	.001350	.005400	.180000	.005400	.010800	.030000	.090000	.004050	.090000	.002700	.001350	.090000	.004050
.100000	.100000	.001667	.006667	.200000	.006667	.013333	.033333	.100000	.005000	.100000	.003333	.001667	.100000	.005000
.120000	.120000	.002400	.009600	.240000	.009600	.019200	.040000	.120000	.007200	.120000	.004800	.002400	.120000	.007200
.125000	.125000	.002604	.010417	.250000	.010417	.020833	.041667	.125000	.007813	.125000	.005208	.002604	.125000	.007813
.150000	.150000	.003750	.015000	.300000	.015000	.030000	.050000	.150000	.011250	.150000	.007500	.003750	.150000	.011250
.180000	.180000	.005400	.021600	.360000	.021600	.043200	.060000	.180000	.016200	.180000	.010800	.005400	.180000	.016200
.200000	.200000	.006667	.026667	.400000	.026667	.053333	.066667	.200000	.020000	.200000	.013333	.006667	.200000	.020000
.240000	.240000	.009600	.038400	.480000	.038400	.076800	.080000	.240000	.028800	.240000	.019200	.009600	.240000	.028800
.250000	.250000	.010417	.041667	.500000	.041667	.083333	.083333	.250000	.031250	.250000	.020833	.010417	.250000	.031250
.300000	.300000	.015000	.060000	.600000	.060000	.120000	.100000	.300000	.045000	.300000	.030000	.015000	.300000	.045000
.360000	.360000	.021600	.086400	.720000	.086400	.172800	.120000	.360000	.064800	.360000	.043200	.021600	.360000	.064800
.400000	.400000	.026667	.106667	.800000	.106667	.213333	.133333	.400000	.080000	.400000	.053333	.026667	.400000	.080000
.420000	.420000	.029400	.117600	.840000	.117600	.235200	.140000	.420000	.088200	.420000	.058800	.029400	.420000	.088200
.480000	.480000	.038400	.153600	.960000	.153600	.307200	.160000	.480000	.115200	.480000	.076800	.038400	.480000	.115200
.500000	.500000	.041667	.166667	1.000000	.166667	.333333	.166667	.500000	.125000	.500000	.083333	.041667	.500000	.125000

5. Application to High-Speed Computors

For this application, it is more convenient to introduce the quantities

$$hz_{2n}=Z_{2n}, \qquad \frac{1}{3}h^2f_{2n}=F_{2n}, \qquad \frac{4}{3}h^2f_{2n+1}=F_{2n+1}.$$

From our formulas it is easy to deduce that only four cells are needed to store the values of y, Z, and F. We shall give here a possible arrangement of the calculation so as to have only one multiplication when the F's are computed.

Thus for the general step, if in the memory cells, P, Q, R, S, we have at a certain moment the following situation [4]

$$(P)=y_0, \qquad (Q)=Z_0, \qquad (R)=F_0, \qquad (S)=F_{-1},$$

the following five orders

$$(Q)+(R)\to Q, \quad (P)+(Q)\to P, \quad \frac{1}{8}(S)\to S, \quad (R)-(S)\to S, \quad (P)+(S)\to S,$$

put y_1 in S or in the y cell of the subroutine corresponding to (1). This subroutine produces F_1, which is stored in S. The two orders

$$(Q)+(S)\to Q, \qquad (P)+(Q)\to P,$$

then put y_2 in P, and the subroutine corresponding to (1) computes F_2, which is then stored in R. Finally, the order

$$(Q)+(R)\to Q,$$

puts Z_2 in Q.

To start the computation the method (b) is preferable because once the backward step

$$y_{-1}=y_0-Z_0+\frac{3}{2}F_0$$

has been made, we immediately enter the general routine.

6. Change of Interval

Because f_{-1} needs only to be of first order in (6), there is no difficulty in changing the interval from h_1 to h_2 for the value x_0 of the independent variable. For, if $\overline{f_{-1}}$ denotes the value of f for the last step ($x=x_0-h_1$) and f_{-1}, the value of f which is needed ($x=x_0-h_2$), we have

$$\frac{\overline{f_{-1}}-f_0}{h_1}=\frac{f_{-1}-f_0}{h_2}. \qquad \{1\}$$

Inserting this in (6) we have

$$y_1=y_0+h_2 z_0-\frac{h_2{}^2}{6}\left(\frac{h_2}{h_1}\right)\overline{f_{-1}}+\frac{2}{3}h_2{}^2\left(\frac{3}{4}+\frac{1}{4}\frac{h_2}{h_1}\right)f_0. \qquad \{3\} \qquad (12)$$

In this form, the quantities in the parenthesis are multipliers of the coefficients of (6) for a new interval h_2.

The formula (8) may be deduced from (12) with the particular value $h_1=-h_2$ and with $\overline{f_{-1}}$ replaced by f_1.

7. Error of the Process

Only the error of one general step will be considered. Moreover, since the first derivative has been calculated to the same order as the function itself, i. e., the fourth, only the fifth-order term of the function is of interest. If y_0, z_0, and f_0 are correct, this term is given by the first term neglected when (9) is derived, namely,

$$\frac{2}{45}h^2\Delta^3 f_0, \qquad (13)$$

since f_1 is known to the third order in h, regardless of which of the formulas, (6) or (8) is used

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[4] (X) means contents of cell X.

to compute y_1.   An estimate of the error is thus given by

$$\frac{2}{45} h^5 \left(\frac{d^3 f}{dx^3}\right)_0 = \frac{2}{45} h^5 \left(\frac{d^5 y}{dx^5}\right)_0. \tag{14}$$

However, it is (13) that provides a practical method of estimating the total error.

To check the computation, two methods may be used.

(a) When a first integral of the equation or of the set of equations is known, this may be used at each step as a check because z has been computed.   But confidence in this as a check should not be too great.   Although, if the integration is part of a larger program, this check will be in general sufficient.

(b) If an isolated integration has to be done, greater care may be needed.   The following procedure is then proposed.   Recompute y_1 (which is known with third-order accuracy) by means of the interpolation formula (11) considered backward, so as to use y_2, z_2, and f_2:

$$y_1^* = y_2 - h z_2 + \frac{1}{24} h^2 (-f_0 + 6 f_1 + 7 f_2). \tag{15}$$

The difference is, for the general step, approximately the first neglected term in (6),

$$y_1^* - y_1 = \frac{1}{8} h^2 \Delta^2 f_{-2} = \frac{1}{8} h^4 \left(\frac{d^4 y}{dx^4}\right)_0 \tag{16}$$

and should be small and vary slowly.

The accuracy of the calculation may also be deduced from the comparison of the differences of $y_1^* - y_1$ for two consecutive steps,

$$(y_1^* - y_1)_{2n+2} - (y_1^* - y_1)_{2n} = \frac{1}{8} h^4 \cdot 2h \left(\frac{d^5 y}{dx^5}\right)_0 \qquad n > 0, \tag{17}$$

which is 8/45, the allowed error.   The variation of $y_1^* - y_1$ from one step to the other must therefore remain smaller than the 45/8 of the allowed error for each step.

8. Comparison With Other Methods

It is not our intention to make a detailed comparison here with similar methods—ordinary step by step method, Gauss-Jackson method, Runge-Kutta method.   This task is very delicate, and it is necessary to take care of the higher order terms neglected, the precision needed, and the purpose of the integration.

But we should like to draw attention to the fact, that in most of the other step-by-step methods, predictor and corrector formulas are used for the same value of the independent variable; here, a formula of the corrector type (9) permits us to advance.   Moreover, the advantages are evident—it is easy to start the integration, and there is no problem in changing the interval.

However, since it is possible to make a comparison with the Runge-Kutta method, we should like to develop this point a little more.   It will be seen that the proposed method possesses some of the advantages of the Runge-Kutta method without having some of its inconveniences (see, for instance, Milne [4]).   The Runge-Kutta method may be characterized by the fact that each step is independent and that functions and derivatives are calculated in general four times for the fourth-order process.   Also, in contrast to the step-by-step processes. a maximum accuracy is not sought for each computation, the process being based on compensation, at the end, of all errors made during the step.   But for the case of differential equations of second order of the type at present under consideration, there is one set of formulas for which only three calculations are needed (see Collatz, p. 33–34), and for which, by accident, the function but not the first derivative is calculated each time with maximum accuracy.   In this case the error obtained by comparison with the value y_2 of the Taylor expansion may be written

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in the form

$$y_2^+ - y_2 = \tfrac{2}{45} h^5 \left[F + 6 \left(\frac{\partial f}{\partial y} \right)_0 D \right] f, \tag{18}$$

as may be deduced from the two formulas following (3.13) of reference [1]. In these formulas we set with $n=2$, $\nu=0$, $q=2$, and replace h by $2h$.

In the case of a single differential equation of type (1) the operators F and D are defined by

$$D = \left(\frac{\partial}{\partial x} \right)_0 + z_0 \left(\frac{\partial}{\partial y} \right)_0,$$

$$F = \left(\frac{\partial}{\partial x} + z \frac{\partial}{\partial y} \right)_0^3 + 3 f_0 D \left(\frac{\partial}{\partial y} \right)_0.$$

For the proposed method, (14) may be written with the same notation

$$y_2^* - y_2 = \tfrac{2}{45} h^5 \left[F + \left(\frac{\partial f}{\partial y} \right)_0 D \right] f. \tag{19}$$

Having made this remark, we may now point out that the new method also subdivides the process in steps. These steps are not independent, but the dependence is small (first order only on the second derivative), and because of this small dependence, only two computations are needed instead of three without making the change of interval difficult.

It appears also from a comparison of (18) and (19) that the function is better approximated in general, than with the Runge-Kutta method. This is not the case for the first derivative, which is determined in the Runge-Kutta method with fifth-order accuracy; however, this fifth-order accuracy may be completely illusory.

Finally, we should like to point out that the fourth-order interpolation formula (11) bears a great resemblance, to an analogous formula developed by Lemaitre for the Runge-Kutta methods [3].

9. Example

This method has been used principally for differential equations arising in dynamical problems with two degrees of freedom. Therefore, we shall give an example of this kind that is taken from the problem of primary cosmic rays (cf. references of [2]).

The equations written with the above notations are

$$\frac{d^2 y_1}{dx^2} = a e^{2y_1} - e^{-y_1} + e^{-2y_1} \cos^2 y_2$$

$$\frac{d^2 y_2}{dx^2} = (e^{-2y_1} \cos^2 y_2 - 1 - \tan^2 y_2) \tan y_2,$$

and the first integral is

$$\left(\frac{dy_1}{dx} \right)^2 + \left(\frac{dy_2}{dx} \right)^2 = a e^{2y_1} - 1 - \tan^2 y_2 + 2 e^{-y_1} - e^{-2y_1} \cos^2 y_2.$$

Table 2 presents the computation for the initial conditions

$$y_{1,0} = .448080, \quad y_{2,0} = 0.000000, \quad y'_{1,0} = 0.000000, \quad y'_{2,0} = 0.206279.$$

The value $a = 0.070598$ is deduced from the first integral.

The method (a) of section 4 was used for starting. The results in A were obtained by using $h = 0.2$ and retaining six decimal places. The results in B were obtained by using $h = 0.4$ and retaining five decimal places.

TABLE 2.

Case A

x	y_1	y_2	f_1	f_2	z_1	z_2	C_1	C_2	E_1	E_2	S
0.0	0.448080_0	0.000000_0	-0.057742	-0.000000	0.000000_0	0.206279_1	--------	--------			0
.2	$.446925$	$.041256$	$-.058631$	$-.024492$							
.2	$.446919$	$.041093$	$-.058627$	$-.024394$			3	0	--------		
.4	$.443413_5$	$.081210_6$	$-.061221$	$-.048620$	$-.023564_7$	$.196532_7$	--------		0	0	0
.6	$.437469$	$.119383$	$-.065349$	$-.072382$			-14	2			
.8	$.428869_7$	$.154666_8$	$-.070734$	$-.095146$	$-.049788_2$	$.167646_3$	--------		1	1	0
1.0	$.417462$	$.186141$	$-.076969$	$-.116085$			-6	8			
1.2	$.402963_2$	$.212996_9$	$-.083571$	$-.134105$	$-.080600_4$	$.121406_7$			1	2	0
1.4	$.385128$	$.234476$	$-.089941$	$-.147896$			0	19			
1.6	$.363697_6$	$.250095_7$	$-.095417$	$-.156251$	$-.116517_4$	$.062610_4$			1	2	0

Case B

x	y_1	y_2	f_1	f_2	z_1	z_2	C_1	C_2	E_1	E_2	S
0.0	0.44808_9	0.00000_0	-0.05774	-0.00000	0.00000_0	0.206279	--------	--------			0
.4	$.44346$	$.08251$	$-.06130$	$-.04943$							
.4	$.44337$	$.08119$	$-.06123$	$-.04861$			4	1	--------		
.8	$.42885_9$	$.15465_1$	$-.07073$	$-.09514$	$-.04978_5$	$.16767_1$	--------		1	2	0
1.2	$.40303$	$.21287$	$-.08354$	$-.13402$			-9	9			
1.6	$.36366_5$	$.25005_2$	$-.09541$	$-.15621$	$-.11649_0$	$.06268_2$			3	6	2
2.0	$.30912$	$.26204$	$-.10036$	$-.15266$			9	52			
2.4	$.23888_6$	$.25009_7$	$-.09175$	$-.12404$	$-.19496_9$	$-.05610_3$			5	0	4
2.8	$.15379$	$.21937$	$-.06102$	$-.07788$			41	46			
3.2	$.06010_6$	$.17624_0$	$-.00258$	$-.03068$	$-.24009_1$	$-.11826_6$			4	-12	13

C_1 and C_2 are the fourth-order verification terms $y_{1,1}^* - y_{1,1}$ and $y_{2,1}^* - y_{2,1}$, computed by (16). E_1 and E_2 are the estimates of error deduced from (13). S is the error in the first integral. The quantities C_1, C_2, E_1, E_2, and S are to be multiplied by 10^{-6} in case A and by 10^{-5} in case B.

10. Remarks

(1). It should be noted that (17) is not true for $n=0$, i. e., for the first two steps; for, instead of (6), (8) was used, for which

$$y_1^* - y_1 = -\tfrac{1}{24} h^2 \Delta^2 f_0.$$

By comparison with (16) it appears that the first C is about minus one-third times the second one.

(2). One extra figure is used for $y_{i,2n}$ and $z_{i,2n}$ $(i=1,2)$ to lessen the rounding-off error; this changes very little in the computation, except that the second term in (9) must be written

$$\left(\frac{2h}{10}\right)(10z_0).$$

11. References

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