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A Note on the Numerical Integration of Differential Equations[1]

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An integration method for ordinary differential equations is developed, in which the approximation formulae contain derivatives of higher order than those contained in the differential equation itself. The method is particularly useful for linear differential equations. Numerical examples are given for Bessel's differential equation.

I. Introduction

The object of this note is to present a method for the numerical integration of ordinary differential equations that appears to possess rather outstanding advantages when applied to certain types of equations. The equations to which the method most readily applies are those for which it is possible to obtain, in comparatively simple form, expressions for two additional derivatives. That is, for an equation of n-th order

$$y^{(n)}=f(x,y,y',\ldots,y^{(n-1)}),$$

we obtain by differentiation expressions for $y^{(n+1)}$ and $y^{(n+2)}$. If these expressions are not so involved as to make the labor of substitution prohibitive, then the method here proposed is applicable.

The advantages claimed for the process are:

(1) The start of the integration is accomplished by the same formulas that are used in the regular routine of the process, so that no special formulas or procedures are required in order to get the computation underway.

(2) Each step of the integration makes use of only two lines of the computation, whereas a method employing differences and having a comparable degree of accuracy would require five lines in the computation.

(3) A change in the length of step for step-by-step integration is often necessary as the integration proceeds. Such a change can be more readily made in this process than where five-line formulas of integration are employed.

(4) The coefficients occurring in the formulas are simpler than those in comparable five-line quadrature formulas, so that the machine calculation is not at all complicated.

The most obvious disadvantage of the process is that it requires the calculation of two additional derivatives at each step, and the labor of substitution in certain instances may be excessive. In such cases this method is not recommended. On the other hand, for equations of simple analytical form, and particularly for linear differential equations, it should prove valuable.

II. Derivation of Formulas

Let x_0 and x_1, where $x_1-x_0=h$, be two values of the independent variable x, and let y_0, y_0', etc.. $y_1 y_1'$ etc., be the corresponding values of $y, y', \ldots$ Assuming that y has a continuous derivative of order 7 we may express y, y', y'', and y''' by Taylor's series with remainder term, as follows:

$$y_1=y_0+hy_0'+\frac{h^2y_0''}{2!}+\frac{h^3y_0^{(3)}}{3!}+\frac{h^4y_0^{(4)}}{4!}+\frac{h^5y_0^{(5)}}{5!}+\frac{h^6y_0^{(6)}}{6!}+R_1, \tag{1}$$

$$hy_1'=hy_0'+h^2y_0''+\frac{h^3y_0^{(3)}}{2!}+\frac{h^4y_0^{(4)}}{3!}+\frac{h^5y_0^{(5)}}{4!}+\frac{h^6y_0^{(6)}}{5!}+R_2, \tag{2}$$

$$h^2y_1''=h^2y_0''+h^3y_0^{(3)}+\frac{h^4y_0^{(4)}}{2!}+\frac{h^5y_0^{(5)}}{3!}+\frac{h^6y_0^{(6)}}{4!}+R_3, \tag{3}$$

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$$h^3y_1''' = h^3y_0^{(3)} + h^4y_0^{(4)} + \frac{h^5y_0^{(5)}}{2!} + \frac{h^6y_0^{(6)}}{3!} + R_4, \tag{4}$$

$$y_2 = y_0 + 2hy_0' + \frac{4h^2y_0''}{2!} + \frac{8h^3y_0^{(3)}}{3!} + \frac{16h^4y_0^{(4)}}{4!} + \frac{32h^5y_0^{(5)}}{5!} + \frac{64h^6y_0^{(6)}}{6!} + R_5. \tag{5}$$

From the four equations (1, 2, 3, and 4), the three quantities $y_0^{(4)}$, $y_0^{(5)}$, and $y_0^{(6)}$ may be eliminated, and the resulting equation can be rearranged so as to give

$$y_1 - y_0 = \frac{h}{2}(y_1' + y_0') - \frac{h^2}{10}(y_1'' - y_0'') + \frac{h^3}{120}(y_1''' + y_0''') + R_6. \tag{6}$$

It may be shown by a separate investigation[3] that

$$R_6 = \frac{-h^7y^{(7)}(s)}{100{,}800},$$

in which $x_0 < s < x_1$.

In a similar manner from eq 1 to 5 we may derive

$$y_2 - 2y_1 + y_0 = 7h(y_1' - y_0') - 3h^2(y_1'' + y_0'') + \frac{h^3}{12}(11y_1''' - 5y_0''') + \frac{210h^7y^{(7)}(s)}{100{,}800}, \tag{7}$$

with s in the interval $x_0 < s < x_2$. These are the required formulas.

III. Application to Equations of First Order

Let the given differential equation be

$$y' = f(x,y). \tag{8}$$

Differentiation gives

$$y'' = f_x(x,y) + f_y(x,y)y', \tag{9}$$

and

$$y''' = f_{xx}(x,y) + 2f_{xy}(x,y)y' + f_{yy}(x,y)y'^2 + f_y(x,y)y''. \tag{10}$$

Let the given initial values be x_0, y_0. Then from eq 8, 9, and 10 in succession we obtain y_0', y_0'', y_0''', giving the first line of the computation

$$x_0 \quad y_0 \quad y_0' \quad y_0'' \quad y_0'''.$$

To proceed we assume a trial value for y_1. A fairly good trial value is provided by

$$y_1 = y_0 + hy_0' + \frac{h^2y_0}{2!} + \frac{h^3y_0'''}{3!}.$$

Next with x_1, and the trial value y_1, we obtain trial values for y_1', y_1'', y_1''' from eq 8, 9, and 10 and have the trial line for x_1:

$$x_1 \quad y_1 \quad y_1' \quad y_1'' \quad y_1'''.$$

Now using eq 6 we secure an improved value of y_1, compute y_1', y_1'', y_1''', from eq 8, 9, and 10, recalculate y_1 by 2, (eq 6), and repeat this sequence of steps until no change occurs in the value obtained for y_1. This is taken as correct, and we have two lines of the computation:

$$\begin{matrix} x_0 & y_0 & y_0' & y_0'' & y_0''', \\ x_1 & y_1 & y_1' & y_1'' & y_1'''. \end{matrix}$$

We are now in a position to use formula 7 in order to calculate a trial value for y_2. Then trial values of y_2', y_2'', y_2''' are obtained from eq 8, 9, and 10, and we leave the trial line:

$$x_2 \quad y_2 \quad y_2' \quad y_2'' \quad y_2'''.$$

Formula 6 (with subscripts advanced by 1) gives an improved value for y_2. If the "improved" value of y_2 is different from the "trial" value of y_2, it will be necessary to recompute y_2', y_2'', y_2''' and apply eq 6 again, repeating these steps until no further change occurs. At this stage we have completed three lines of the computation:

$$\begin{matrix} x_0 & y_0 & y_0' & y_0'' & y_0''', \\ x_1 & y_1 & y_1' & y_1'' & y_1''', \\ x_2 & y_2 & y_2' & y_2'' & y_2'''. \end{matrix}$$

Subsequent lines of the calculation are obtained by exactly the same steps as were used to get y_2.

IV. Discussion of the Process

This completes the description of the process for the case of equations of the first order. Some comments of a practical nature are, however, pertinent.

(1) Obviously, the error in y at any step due to the use of the approximate formula 6 is bounded by the quantity

$$E = \frac{h^7M}{100{,}800}, \tag{11}$$

[3] W. E. Milne, The remainder in linear methods of approximation, J. Research NBS **43**, 501 (1949) RP2042.

in which $M=\max|y^{(7)}|$ in the interval covered by the step. Supposing for the moment that M is a known constant, we see that the above equation connects the magnitude of the error E with the length of the step-interval h.

If, for example, the problem in question requires that y be obtained accurately to a specified number of decimal places, eq 11 enables us to select an appropriate value of h that will secure this accuracy. On the other hand, if we have already decided on the value of h, eq 11 will tell us how many decimals in the result may be regarded as correct.

(2) Actually, M is rarely constant from step to step, and moreover the value of M is unknown since it is ordinarily utterly impractical to calculate the value of the seventh derivative of y at each step. However, a crude estimate (which actually proves to be sufficiently satisfactory) may be made as follows: Assume that the calculation has been performed correctly to the nth step so that we have the correct values of the line

$$x_n \qquad y_n \qquad y_n' \qquad y_n'' \qquad y_n''',$$

a trial value $\overline{y}_{n+1}$ is obtained by eq 7. A final value of y_{n+1} is obtained by eq 6, repeated if necessary. Now the error of $\overline{y}_{n+1}$ is

$$\frac{210h^7y^{(7)}(s)}{100{,}800},$$

whereas that of y_{n+1} is

$$-\frac{h^7y^{(7)}(s')}{100{,}800}+e,$$

e being the error produced in y_{n+1} by the errors in y_{n+1}', y_{n+1}'', y_{n+1}''', these latter being due to the error of y_{n+1}. In actual practice, if the process is rapidly enough convergent for practical use, the error e must be much smaller than the error in $\overline{y}_{n+1}$. Hence, we may neglect e. Then

$$\overline{y}_{n+1}-y_{n+1}=\frac{210h^7y^{(7)}(s)}{100{,}800}+\frac{h^7y^{(7)}(s')}{100{,}800}.$$

If we ignore the fact that $y^{(7)}(s)$ and $y^{(7)}(s')$ are not exactly the same, we may add the terms on the right, divide by 211, and obtain

$$\text{Error of } y_{n+1}=-\frac{h^7y^{(7)}(s)}{100{,}800}=\frac{y_{n+1}-\overline{y}_{n+1}}{211}.$$

Although the foregoing reasoning seems very crude, the final formula

$$\text{Error of } y_{n+1}=\frac{y_{n+1}-\overline{y}_{n+1}}{211},$$

proves to be not only simple in application but actually quite reliable in determining how many significant figures of the result can be trusted.

(3). At each step of the computation the quantity $c_n=y_n-\overline{y}_n$ should be recorded in a separate column. This column of c's is used for several purposes.

(a) As long as the c's vary regularly and have significant figures only in the last two places retained, we proceed with the computation in reasonable confidence that all is well.

(b) A sudden fluctuation in the c's suggests that a computational mistake has been made, and the lines involved should be rechecked.

(c) If the c's increase to the point of affecting the last three places retained, then either the interval, h, should be shortened, or one less place should be retained.

(d) The necessity for recomputing y_{n+1}', y_{n+1}'', y_{n+1}''' can frequently be obviated by estimating c_{n+1} from the known values c_{n-2}, c_{n-1}, c_n and adding it to the trial value $\overline{y}_{n+1}$ *before* computing y_{n+1}', y_{n+1}'', y_{n+1}'''. If the estimate is sufficiently accurate, no recomputation is required.

(4). The foregoing discussion applies only after the computation is under way and does not give any clue to the accuracy of y_1. We would, of course, like to decide on the value of h and on the number of decimal places before starting the computation. This requires that we calculate $y_0^{(7)}$ from the differential equation and the initial values.

V. Equations of Higher Order

The modifications required to apply the process to equations of second or higher order are slight. In the case of an equation of second order, for example, the routine (after the start has been made) is as follows:

Predict y_2' by eq 7 modified as follows:

$$y_2'-2y_1'+y_0'=7h(y_1''-y_0'')-3h^2(y_1'''+y_0''')+\frac{h^3}{12}(11y_1^{(4)}-5y_0^{(4)}).$$

Predict y_2 by eq 7. Calculate y_2'', y_2''', $y_2^{(4)}$ from the differential equations and the equations obtained by differentiation.

Correct y_2' by

$$y_2'-y_1'=\frac{h}{2}(y_2''+y_1'')-\frac{h^2}{10}(y_2'''-y_1''')+\frac{h^3}{130}(y_2^{(4)}+y_1^{(4)}).$$

Correct y_2 by

$$y_2-y_1=\frac{h}{2}(y_2'+y_1')-\frac{h^2}{10}(y_2''-y_1'')+\frac{h^3}{130}(y_2'''+y_1''').$$

VI. Illustrative Examples

The foregoing method is applied to the second order differential equation

$$xy''+y'+xy=0,$$

with conditions $y=1$, $y'=0$ at $x=0$.

Example 1, below, gives the solution by another method using $h=0.1$. Example 2 uses the present method with $h=0.5$. A comparison of the computation time is given. Example 3 uses the present method with $h=0.1$.

It appears that in example 2 the error of y is about 2 in sixth place, whereas in example 3 the error is occasionally 1 in the tenth place.

A comparison of example 1 and example 2 shows that the new method obtained the value of $J_0(3)$ in only six steps (and more accurately) than the simple method based on Simpson's Rule could secure in 30 steps. Although the labor of substitution per step is much greater for the new method, the reduction in number of required steps more than offsets this extra work, as is shown by a comparison of required times.

Example 3 provides further evidence of the power of the new method. Anyone with experience in numerical solution of differential equations will recognize that to solve Bessel's equation to 10 decimal places in the neighborhood of the orign with step-intervals of length 0.1 requires a pretty accurate method of solution.

Differential equation: $x\dfrac{d^2y}{dx^2}+\dfrac{dy}{dx}+xy=0$

Computation formulas

Predictor: $y'_{n+1}=y'_{n-3}+h[4y''_{n-1}+8/3\ \delta^2y''_{n-1}]$.

Corrector: $y'_{n+1}=y'_{n-1}+h[2y''_n+1/3\ \delta^2y''_n]$.

Derivatives: $y''=-\dfrac{1}{x}\,y'-y$.

Time: 2¼ hr; $h=0.1$

x	y	y'	y''	$\frac{1}{3}\delta^2y'$	$\frac{1}{3}\delta^2y''$	c	c'	True values	
								y	y'
0.2	[a]0.990025	[a]−0.099501	−0.492520	--------	---------	---	---	-------	---------
.3	[a].977626	[a]−.148319	−.483229	0.000370	0.001203	---	---	-------	---------
.4	[a].960398	[a]−.196027	−.470330	.000489	.001166	---	---	-------	---------
.5	[a].938470	[a]−.242268	−.453934	.000603	.001122	---	---	-------	---------
.6	.912005	−.286702 (0)	−.434168	.000714	.001065	0	2	0.912005	−0.286701
.7	.881201	−.328995	−.411208	.000815	.001004	0	0	.881201	−.328996
.8	.846288	−.368843 (2)	−.385234	.000914	.000930	0	1	.846287	−.368842
.9	.807524	−.405949 (8)	−.356470	.001001	.000853	0	1	.807524	−.405950
1.0	.765198	−.440052	−.325146	.001085	.000764	0	0	.765198	−.440051
1.1	.719622	−.470902 (1)	−.291529	.001154	.000674	0	1	.719622	−.470902
1.2	[b].671133 (5)	−.498290	−.255891	.001219	.000574	2	0	.671133	−.498289
1.3	.620086	−.522023 (1)	−.218530	.001269	.000473	0	2	.620086	−.522023
1.4	.566855 (7)	−.541949	−.179749	.001313	.000366	2	0	.566855	−.541948
1.5	.511828	−.557936	−.139871	.001342	.000259	0	0	.511828	−.557937
1.6	.455402 (4)	−.569897	−.099216	.001364	.000146	2	0	.455402	−.569896
1.7	.397985	−.577765 (4)	−.058123	.001372	+.000037	0	1	.397985	−.577765
1.8	.339986 (7)	−.581518 (9)	−.016920	.001371	−.000077	1	−1	.339986	−.581517
1.9	.281819 (20)	−.581157 (6)	+.024053	.001357	−.000184	1	1	.281819	−.581157
2.0	.223890 (2)	−.576726 (7)	.064473	.001334	−.000295	2	−1	.223891	−.576725
2.1	.166607 (8)	−.568292 (1)	.104008	.001298	−.000398	1	+1	.166607	−.568292
2.2	.110361 (3)	−.555964 (5)	.142350	.001255	−.000502	2	−1	.110362	−.555963
2.3	.055540 (1)	−.539872	.179187	.001198	−.000595	1	0	.055540	−.539873
2.4	.002506 (8)	−.520186 (8)	.214238	.001136	−.000689	2	−2	+.002508	−.520185
2.5	−.048384 (3)	−.497093	.247221	.001060	−.000771	+1	0	−.048384	−.497094
2.6	−.096807 (5)	−.470819 (20)	.277891	.000982	−.000852	+2	−1	−.096805	−.470818
2.7	−.142450 (49)	−.441600	.306006	.000890	−.000919	+1	0	−.142449	−.441601
2.8	−.185038 (6)	−.409710 (1)	.331363	.000798	−.000984	+2	−1	−.185036	−.409709
2.9	−.224312	−.375426	.353769	.000694	−.001034	0	0	−.224312	−.375427
3.0	−.260054 (3)	−.339060 (1)	.373074	--------	---------	+1	−1	−.260052	−.339059

[a] Starting values given.

[b] In the column for y and y' appear the corrected values. The digits of the predicted values when different from the corrected are shown in parentheses.

Example 2.

Differential equation: $x\frac{d^2y}{dx^2}+\frac{dy}{dx}+xy=0$

Computation formulas

Predictor: $y'_{n+1}=2y'_n-y'_{n-1}+7h(y''_n-y''_{n-1})-3h^2(y'''_n+y'''_{n-1})+\frac{h^3}{12}(11y^{\mathrm{IV}}_n-5y^{\mathrm{IV}}_{n-1})$

$$y_{n+1}=2y_n-y_{n-1}+7h(y'_n-y'_{n-1})-3h^2(y''_n+y''_{n-1})+\frac{h^3}{12}(11y'''_n-5y'''_{n-1})$$

Corrector: $y'_{n+1}=y'_n+\frac{h}{2}(y''_{n+1}+y''_n)-\frac{h^2}{10}(y'''_{n+1}-y'''_n)+\frac{h^3}{120}(y^{\mathrm{IV}}_{n+1}+y^{\mathrm{IV}}_n)$

$$y_{n+1}=y_n+\frac{h}{2}(y'_{n+1}+y'_n)-\frac{h^2}{10}(y''_{n+1}-y''_n)+\frac{h^3}{120}(y'''_{n+1}+y'''_n)$$

Derivatives: $y''=-\frac{1}{x}y'-y$

$$y'''=-\frac{2}{x}y''-y'-\frac{1}{x}y$$

$$y^{\mathrm{IV}}=-\frac{3}{x}y'''-y''-\frac{2}{x}y'$$

Time: 1¼ hr; $h=0.5$

x	y	y'	y''	y'''	y^{IV}	c	c'	True values y	True values y'
0	[a]1.	[a]0	−0.5	0	0.375	---	---	--------	----------
0.5	0.938470	[a]−0.242268	−.453934	0.181064	.336622	---	---	--------	----------
1.0	[b].765195 (9)	−.440047 (63)	−.325148	.325148	.229798	4	−16	0.765198	−0.440051
1.5	.511826 (31)	−.557934 (5)	−.139870	.403210	.077382	5	−1	.511828	−.557937
2.0	.223889 (2)	−.576721 (18)	+.064472	.400304	−.088207	−7	+3	.223891	−.576725
2.5	−.048382 (6)	−.497090 (1)	.247218	.318668	−.231948	−4	−6	−.048384	−.497094
3.0	−.260053 (47)	−.339057 (48)	.373066	.177021	−.324043	6	+3	−.260052	−.339059

[a] Starting values given.
[b] In the column for y and y' appear the corrected values. The digits of the predicted values when different from the corrected are shown in parentheses.

Example 3.

Differential equation: $x\frac{d^2y}{dx^2}+\frac{dy}{dx}+xy=0.$

Computation formulas: (Same as Example 2.).

Computation, $h=0.1$.

	y	y'	y''	y'''	y^{IV}	c	c'	True values	y	y'
0.5	[a]1 -------	[a]0 -------	−0.5 -----	0 -----	0.375 -----	---	---	---	-----------	--------------
.1	[a]0.99750 15621	[a]−0.04993 75260	−.49812 63017	0.03744 79394	.37343 86390	---	---	---	-----------	--------------
.2	.99002 49723	−.09950 08326 (7)	−.49252 08093	.07458 40641	.36876 81738	−0	−1	0.2	0.99002 49722	−0.09950 08326
.3	.97762 62466	−.14831 88162 (6)	−.48323 01926	.11109 92782	.36102 95182	0	−4	.3	.97762 62465	−.14831 88163
.4	.96039 82267	−.19602 65779 (81)	−.47033 17820	.14668 99212	.35029 02625	0	−2	.4	.96039 82267	−.19602 65780
.5	[b].93846 98073 (2)	−.24226 84576 (9)	−.45393 28921	.18106 04114	.33664 42541	−1	−3	.5	.93846 98072	−.24226 84577
.6	.91200 48636 (5)	−.28670 09880 (1)	−.43416 98836	.21392 58273	.32021 07071	−1	−1	.6	.91200 48635	−.28670 09881
.7	.88120 08887	−.32899 57415 (6)	−.41120 69723	.24501 43928	.30113 31217	0	−1	.7	.88120 08886	−.32899 57415
.8	.84628 73528 (7)	−.36884 20461 (2)	−.38523 47952	.27406 98431	.27957 79988	−1	−1	.8	.84628 73528	−.36884 20461
.9	.80752 37982 (0)	−.40594 95461 (2)	−.35646 87470	.30085 36525	.25573 33411	−2	−1	.9	.80752 37981	−.40594 95461
1.0	.76519 76866 (0)	−.44005 05858 (9)	−.32514 71008	.32514 71008	.22980 69700	−6	−1	1.0	.76519 76866	−.44005 05857

[a] Starting values given.
[b] In the column for y and y' appear the corrected values. The digits of the predicted values when different from the corrected are shown in parentheses.

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