ON THE IMPROVEMENT OF ACCURACY IN INTEGRATION*

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1. Introduction. In solving numerically systems of ordinary differential equations in a stepwise manner it is frequently advisable, and certainly economically more efficient, to vary the step size as the integration proceeds. Further, when applying methods of integration that necessitate the computation at the "next" point of a number of approximate values for the unknown functions it may be desirable to employ the different approximations so as to increase the accuracy obtainable.

Both of these ideas are not new, and have been used on occasion previously, though mostly separately.

The scheme proposed here attempts to combine both techniques in a proper manner. The resulting methods are shown to work very effectively on a few critical examples; they are also in general sufficiently simple to be easily applicable to modern high speed computing machines.

2. The integration scheme. Let us assume that the integration problem is of the form

$$y' = f(x, y), \quad y(x_0) = y_0, \quad (1)$$

where y and $f(x, y)$ are column matrices of n components. The associated numerical problem is then of the form

$$Y' = F(x, Y),$$

where Y is a numerical approximation to y , and $F(x, Y)$ differs from $f(x, Y)$ by certain rounding errors which are due to the mode of construction of f from its arguments x, Y . It will, in general, be convenient to denote mathematically exact quantities by small letters, their numerical representatives by corresponding capital letters. Concurrently, it should be recognized that the arithmetical operations involving such numerical approximants are of the "pseudo-arithmetical" type, of necessity introducing certain errors due to unavoidable rounding.

Let us suppose, further, that the solution of the associated numerical problem has proceeded through a sequence of points $x_1, x_2, \dots, x_{k-1}$ to a point x_k , so that the last step size employed was $h = x_k - x_{k-1}$.

The integration scheme then consists simply in securing two approximations V_1, V_2 at $x_{k+1} = x_k + h$, and then utilizing their difference

$$\delta Y = V_1 - V_2 \quad (2)$$

for the double purpose of a) improving the accuracy of the V_1 , and b) deciding whether or not a change in step size is warranted.

The importance of δY for accuracy considerations is easily recognized. Let the exact value of the solution be denoted by $y(x)$, so that

$$Y_k = y(x_k) + \eta_k; \quad (3)$$

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η_k represents the total error accumulated at x_k . The two approximants V_1 , V_2 are now related to the exact value $y(x_{k+1})$ as follows:

$$V_i = y(x_{k+1}) + e_i, \quad i = 1, 2. \quad (4)$$

To fix the notation let V_2 denote the more exact determination of y at x_{k+1} .

It may be assumed that the exact errors e_i are composed linearly of terms due, respectively, to truncation, accumulation and rounding:

$$e_i = \sum_{\alpha=1} b_{i\alpha} t_\alpha + \sum_{\beta=k, k-1} c_{i\beta} u_\beta + \sum_{\gamma=1} d_{i\gamma} r_\gamma. \quad (5)$$

Since $\delta Y = e_1 - e_2$ it is then clear that a relationship of the form

$$e_2 = a \delta Y + \sum_{\alpha} b'_\alpha t_\alpha + \sum_{\beta} c'_\beta u_\beta + \sum_{\gamma} d'_\gamma r_\gamma \quad (6)$$

must exist. The major part of e_2 , which is easily computed numerically, is

$$E_2 = A \delta Y + \sum_{\alpha} B_\alpha T_\alpha + \sum_{\beta} C_\beta U_\beta. \quad (7)$$

Let the difference between e_2 and E_2 be η_{k+1} . If we now take for the final value of Y at x_{k+1} the quantity

$$Y_{k+1} = V_2 - E_2, \quad (8)$$

then obviously

$$Y_{k+1} = y(x_{k+1}) + \eta_{k+1}.$$

The adjustment of step size may be tied to the magnitude of E_2 , as follows. Suppose it is desired to keep $|e_2| \leq \epsilon$, where $\epsilon > 0$ is prescribed. In general,

$$|E_2| = m\epsilon,$$

where m is some positive number. It is then reasonable to expect these alternatives:

(a) if $m > 1$ shorten h ; (b) if $m < m_0 \ll 1$ enlarge h ; (c) if $m_1 < m \leq 1$, leave h unchanged.

Some of the methods for obtaining δY may be put conveniently into the following two categories:

I. Application of two distinct methods at full step. The "predictor-corrector" techniques [1] are of this type.

II. Application of a particular method first at full step, then at two successive half steps; these may be said to employ "local extrapolation to zero step" [2]. Special cases of each of these categories are considered below.

3. Predictor-corrector method. A good combination is provided by the choice of a low order central difference method for predictor, and Heun's method for corrector. The central difference formula is

$$V_1 = Y_{k-1} + 2hY'_k; \quad (9)$$

its truncation error is $t_1 = (h^3/3)y'''(s_1)$, $x_{k-1} < s_1 < x_{k+1}$. Heun's method, on the other hand, employs the formulas:

$$V_0 = Y_k + hY'_k, \quad (10)$$

$$V_2 = Y_k + (h/2)(Y'_k + V'_0); \quad (11)$$

the truncation error of Eq. (10), which is Euler's method, is $t_0 = (h^2/2)y''(s_0)$, that of Eq. (11) is $t_2 = -(h^3/12)y'''(s_2)$, $x_k < s_0$, $s_2 < x_{k+1}$. It is found that

$$e_1 = -t_1 + 2pu_k + u_{k-1} + \dots, \quad (12)$$

$$e_2 = -t_2 - 2^{-1}pt_0 + (I + p + 2^{-1}p^2)u_k + \dots, \quad (13)$$

where p denotes the matrix of elements $p_{ij} = \partial f_i / \partial y_j$, I is the unit matrix of n th order, and the omitted terms are due to local rounding only. Since $t_1 \approx -4t_2$, above equations result in

$$E_2 = \delta Y - (6T_2 + PT_0) + U_{k+1}, \quad (14)$$

where

$$U_{k+1} = (2I + P^2)U_k - U_{k-1}, \quad (15)$$

and the T_i , P are evaluated at x_{k+1} , V_2 .

Of interest may be the fact that by subtracting Eq. (13) from Eq. (12) there is obtained

$$t_2 = (1/5)[\delta Y - (1/2)pt_0 + (I + p)^{-1}u_k - u_{k-1}];$$

the resulting approximation

$$t_2 \approx \delta Y/5 \quad (16)$$

was previously pointed out by Milne [1], p. 28.

It is clear in general that combinations of formulas having "comparable" truncation errors $c_i h^i y^{(n)}(s_i)$ permit estimates similar to (16). However, combinations not possessing this property may still be useful.

Such a combination is, for example, that composed of formulas (10) and (11). In this case one gets

$$e_1 = -t_0 + (I + p)u_k + \dots,$$

$$e_2 = -t_2 + (I + 2^{-1}p)u_k + 2^{-1}pe_1 + \dots.$$

Replacing in the latter equation e_1 by $e_2 + \delta Y$ there results

$$E_2 = (2I - P)^{-1}[P \delta Y - 2T_2] + U_{k+1}, \quad (17)$$

with

$$U_{k+1} = (2I - P)^{-1}(2I + P)U_k. \quad (18)$$

Other predictor-corrector combinations may be analyzed in the same vein.

4. Local extrapolation. For purposes of illustration let us apply the technique of local extrapolation to Heun's method. For the first approximation, then, as by Eqs. (10) and (11),

$$V_1 = Y_k + (h/2)(Y'_k + V'_0).$$

Next, let ξ_k bisect the interval $\langle x_k, x_{k+1} \rangle$, and let us define $z_k = y(\xi_k)$, $w = h/2$. The second approximation V_2 is then obtained thus:

$$\begin{aligned} W_0 &= Y_k + wY'_k, \\ W_1 &= Y_k + (w/2)(Y'_k + W'_0), \\ W_2 &= W_1 + wW'_1, \\ V_2 &= W_1 + (w/2)(W'_1 + W'_2). \end{aligned} \quad (19)$$

By Eq. (13), where e_2 now becomes e_1 ,

$$e_1 = -t_2 - 2^{-1}pt_0 + (I + p + 2^{-1}p^2)u_k + \dots$$

Consequently,

$$\begin{aligned} e'_1 &\equiv W_1 - y(\xi_k) \\ &= -\tau_2 - 2^{-1}\pi\tau_1 + (I + \pi + 2^{-1}\pi^2)u_k + \dots, \end{aligned}$$

where the τ_i and η differ from the t_i and p only in that h is replaced by w . Since, therefore,

$$\pi \approx 2^{-1}p, \quad \tau_1 \approx 2^{-2}t_1, \quad \tau_2 \approx 2^{-3}t_2,$$

it follows that

$$8e'_1 \approx e_1 + (7I + 3p + 2^{-1}p^2)u_k + \dots \quad (20)$$

On the other hand, a short calculation shows that

$$e_2 = (2I + 2^{-1}p + 2^{-3}p^2)e'_1 - (I + 2^{-1}p + 2^{-3}p^2)u_k + \dots$$

Therefore, using Eq. (20) while neglecting terms of order p^2 , there is obtained

$$E_2 = (1/3)(I + P/3) \delta Y + U_{k+1}, \quad (21)$$

where

$$U_{k+1} = (I + P)u_k.$$

It is not difficult to extend this discussion to more accurate integration procedures. In doing this let us restrict ourselves to a single differential equation

$$y' = f(x, y), \quad y(x_0) = y_0,$$

and utilize the fact that most integration methods are equivalent to forms [3]

$$Y_k^{(i)} = F_i(x_k, Y_k, Y'_k, \dots, Y_k^{(i-1)}), \quad i = 1, 2, \dots, N, \quad (22)$$

$$V_0 = Y_k + hY'_k + \dots + [h^{N-1}/(N-1)!]Y_k^{(N-1)},$$

$$\begin{aligned} V_1 &= \sum_{i=0}^r G_{0i}Y_{k-i} + h\left(G_1V'_0 + \sum_{i=0}^r G_{1i}Y'_{k-i}\right) + \dots \\ &\quad + h^N\left(G_NV_0^{(N)} + \sum_{i=0}^r G_{Ni}Y_{k-i}^{(N)}\right). \end{aligned} \quad (23)$$

Here the g_{ii} are constants which in general depend on the range r of points x_{k-i} to the left of x_k , and N indicates the degree of the polynomials for which the method is exact.

Proceeding in the same manner as described above one obtains eventually

$$e_2 = \delta Y \frac{1 + g_{00}}{2^{N+1} - 1 - g_{00}} \left[1 + p \frac{2^N(g_1 + g_{10})}{(2^{N+1} - 1 - g_{00})(1 + g_{00})} \right] + \dots \quad (24)$$

In those methods where $g_{00} = 1$, such as Euler's, Heun's, Adam's, Gregory's, etc., Eq. (24) becomes

$$e_2 = \frac{\delta Y}{2^N - 1} \left[1 + p(g_1 + g_{10}) \frac{2^{N-2}}{2^N - 1} \right] + \dots \quad (25)$$

In Heun's method, for example,

$$(g_{00}, g_1, g_{10}) = (1, 1/2, 1/2), \quad N = 2,$$

and consequently

$$E_2 = (1/3)(1 + P/3) \delta Y + \dots,$$

which agrees with the principal part of Eq. (21).

5. Numerical example. The technique described above was tried out on the simple case of the differential equation

$$y' = y^2, \quad (26)$$

whose solution is $y(x) = (c - x)^{-1}$. For the integration the predictor-corrector combination of Euler-Heun was used:

$$\begin{aligned} V_1 &= Y_k + hY'_k, & V_2 &= Y_k + (h/2)(Y'_k + V'_1), \\ E_2 &= (2 - P)^{-1}(P \delta Y - 2T_2) + U_{k+1}, & U_{k+1} &= (2 - P)^{-1}(2 + P)U_k, \\ Y_{k+1} &= V_2 - E_2. \end{aligned} \quad (27)$$

For our problem (26),

$$P = 2hY_2, \quad T_2 = -(h^3/2)Y_2^4.$$

A. Initial Condition $y(0) = 1$.

Starting with $y(0) = 1$ it was desired to obtain the solution in the interval $0 \leq x < 1$ to an accuracy of three decimal places.

The results of a number of integrations performed with Heun's method modified in a variety of ways are shown in Tables 1 and 2.

TABLE 1
Improvement In Accuracy. Comparisons

x	(1) Y (No Corr.)	(2) Error	(3) Y (One Corr.)	(4) Error	(5) Y (Two Corr.)	(6) Error
0	1.000000	0.10^{-6}	1.000000	0.10^{-6}	1.000000	0.10^{-6}
.04	1.041632	-35	1.041664	-3	1.041667	0
.08	1.086878	-79	1.086950	-7	1.086957	0
.12	1.136229	-135	1.136352	-12	1.136363	-1
.16	1.190270	-206	1.190458	-18	1.190474	-2
.20	1.249702	-298	1.249972	-28	1.249996	-4
.24	1.315373	-416	1.315749	-40	1.315782	-7
.28	1.388318	-571	1.388831	-58	1.388875	-14
.32	1.469815	-773	1.470506	-83	1.470565	-23

TABLE 2
Adjustment In Step Size

x	(1) Y	(2) δY	(3) P	(4) T_2	(5) E_2	(6) E_2^*	(7) Error
0	1.000000	0.10^{-6}	8000.10^{-5}	(-32.10^{-6})	0.10^{-6}	0.10^{-6}	0.10^{-6}
.04	1.041667	-1632	8333	-38	-35	114	0
.32	1.470565	-4406	17635	-150	-125	343	-23
.34	1.515129	-1291	60604	-21	-22	66	-23
.36	1.562479	-1413	62498	-24	-25		-21
.60	2.499982	-5528	99994	-156	-140	469	-18
.61	2.564086	-1582	51281	-22	-23	67	-17
.62	2.631564	-1708	52631	-24	-25		-15
.76	4.166679	-6528	83331	-151	-139	454	+12
.765	4.255334	-1827	42553	-20	-22	64	15
.770	4.347844	-1947	43478	-22	-24		18
.860	7.143004	-8343	71429	-163	-154	492	147
.8625	7.272882	-2298	36364	-22	-24	68	155
.8650	7.407570	-2426	37038	-24	-25		163
.9000	10.000355	-5875	50001	-78	-78	244	355

1. No corrections. For the accuracy required it is clearly sufficient to start with $h = 0.04$. Using Heun's method without any modifications there are obtained the values listed in column (1) of Table 1; the errors, shown in column (2), are seen to exceed the tolerance $\epsilon = 5.10^{-4}$ already at $x = 0.28$.

2. One correction. Next the integration was carried out utilizing the expression for E_2 without the term U_{k+1} . The results are exhibited in column (3), the errors in column (4). This modification reduces the errors to about one tenth of their previous values.

3. Two corrections. The inclusion of U_{k+1} in E_2 produced the results shown in column (5); the errors, in column (6), are reduced further considerably.

The continuation of column (5), together with the appropriate adjustment in step size, is shown in Table 2.

The integration interval was cut whenever the quantity

$$E_2^* = (2 - P)^{-1} [|P \delta Y| + 2 |T_2| + (2 + P) |U_k|] \quad (28)$$

exceeded 5.10^{-4} ; this occurred at $x = 0.36, 0.62, 0.77$ and 0.865 . At $x = 0.9$ the step size was $h = 0.0025$, the error $\eta = .000355$. Use of this step size from the beginning would require 360 lines of integration, while the computation shown in Table 2 necessitated only about one fifth of that number.

4. Use of δY for step adjustment. Instead of watching E_2^* for adjusting the step size, the quantity δY could be used for this purpose, as suggested by Milne [1]. Cutting the interval whenever δY exceeded 0.0025 , which occurred at $x = 0.20, 0.48, 0.67$, the error increased to $.000496$ already at $x = 0.69$, so that the use of E_2^* seemed superior, at least in this example.

5. The approximation $E_2 \approx T_2$. Inspection of columns (4) and (5) shows that $E_2 \approx T_2$, which is to be expected. If this assumption $E_2 \approx T_2$ is introduced into Eq. (27), there results

$$E_2 = (4 - P)^{-1} P \delta Y. \quad (29)$$

An integration based on this formula, with changes of interval whenever $|P\delta Y| < 5.10^{-4}$, produced an error of -0.000478 at $x = 0.78$. A graphical illustration of the various techniques is also given in Fig. 1.

FIG. 1

Further inspection of Table 1 shows that the application of the unmodified Heun method leads to an error of -693.10^{-6} at $x = 0.60$. It is of interest to note that this error is quite closely approximated by the error propagation theorem derived in [3]. It was shown there that the total accumulated error for Heun's method is

$$\Omega_k \approx [-1 + 2^{-1}p, h] \sum_{i=1}^k \lambda^{k-i} \begin{bmatrix} -T_i + r_1 \\ r_2 \end{bmatrix}, \quad (30)$$

with

$$\lambda = \Lambda/D = (g_{00} + pg_{10})/(1 - pg_1) = (1 + 2^{-1}p)/(1 - 2^{-1}p).$$

In our example $r_1, r_2 \approx 5.10^{-6}$, so that the contributions due to these errors may be neglected. Consequently,

$$\Omega_k \approx \frac{2-p}{2} \left(\frac{2+p}{2-p} \right)^k \sum_{i=1}^k \left(\frac{2-p}{2+p} \right)^i T_i. \quad (31)$$

Using in (31) the average value $2^{-1}(p_1 + p_k)$ for p , there is obtained for the total accumulated error at $x = 0.60$ the value -723.10^{-6} , which differs from the exact error -693.10^{-6} by only about 4%.

B. Initial Condition $y(2) = -1$. The purpose of this computation is to illustrate the possibility of continual enlargement of h without the loss of accuracy. The results are shown in Table 3. First Heun's method without any modification was applied, at a

TABLE 3
Adjustment In Step Size

	(1)	(2)	(3)	(4)	(5)	(6)	(7)
x	Y (No Corr.)	Error	Y (Two Corr.)	T_2	E_2	E_2^*	Error
2.00	-1.000000	0.10^{-6}	-1.000000	(-32.10^{-6})	0.10^{-6}	0.10^{-6}	0.10^{-6}
2.04	-.961568	-30	-.961538	-24	-30	86	0
2.44	-.694567	-123	-.694447	-7	-7	25	-3
2.52	-.658018	-123	-.657893	-48	-57	175	2
2.60	-.625121	-121	-.625996	-39	-46		4
3.40	-.416751	-84	-.416664	-8	-8	25	3
3.56			-.390618	-48	-59	1777	7
3.72			-.367638	-37	-45		9
5.16			-.240379	-7	-7	25	6
5.48			-.223205	-41	-51	140	9
5.80			-.208323	-31	-38		10
7.72			-.148801	-8	-9	27	9

constant step of $h = 0.04$. The errors are listed in column (2); since now $p < 0$ the errors tend to damp out.

In the remaining columns (3) to (7) there are again exhibited the computations using the technique described in Eqs. (27). The interval was doubled whenever E_2^* fell below 25.10^{-6} , which occurred at $x = 2.48, 3.48, 5.32, 8.04, \dots$. The error at $x = 7.72$ was 9.10^{-6} , which could hardly have been improved upon even with a constant step size of $h = 0.04$, at a computational labor of 143 lines of integration instead of the 42 needed for Table 3.

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