## A Method for the Numerical Solution of y' = f(x, y) Based on a Self-Adjusting Non-Polynomial Interpolant

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1. Introduction. In a recent paper, [1], the authors considered a class of formulae for the numerical solution of

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

in which the underlying interpolant is a rational function: this is in contrast with classical formulae which are, in general, based on polynomial approximation. With the formulae of [1], the solution of (1) is locally represented by an interpolant which can possess a simple pole, thus affording an improved numerical solution close to a singularity of the theoretical solution of (1). The present paper proposes formulae containing two parameters which control the nature of the basic interpolant; if it is necessary that the interpolant possess a singularity, then one of the parameters controls the position, and the other the nature of the singularity. The value of these parameters are automatically chosen, and revised, during the computation. Thus the method produces an algorithm based on a local interpolant which is automatically adjusted to suit the needs of the particular differential equation whose solution is sought.

Various authors have suggested techniques for enabling numerical methods to cope with a specific known singularity. Krylov [2] discusses the problem in relation to quadrature, and Fox [3] refers to a similar situation in second-order ordinary differential equations. The methods proposed in the present paper do not require previous knowledge of the nature or position of the singularity: indeed, estimates for these quantities are provided by the algorithms.

2. Basic Interpolants. Along the x-axis, consider the points  $x_r$  to be given by

$$x_r = x_0 + rh$$
  $(r = 0, 1, 2, \cdots),$ 

where h is the distance between consecutive points. We assume that the solution of (1) is locally represented in the range  $[x_n, x_{n+1}]$  by the interpolant

(2) 
$$y^*(x) = \sum_{p=0}^{L} a_p x^p + b | A + x |^{N},$$

where  $a_p$ , b, A and N are real, L is a positive integer, and

$$(3) N \in \{0, 1, 2, \cdots, L\}.$$

The L+2 constants b,  $a_p$  ( $p=0,1,\dots,L$ ) are regarded as undetermined coefficients, while A and N are the parameters whose values control the position and nature respectively of any possible singularity of  $y^*$ . If N is negative, then  $y^*$  possesses a singularity at x=-A, but since N is not necessarily integral, the class

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of interpolants corresponding to negative N is wider than that considered in [1]. If N is a positive integer  $\ge L+1$ , then, in either of the intervals x<-A, x>-A,  $y^*$  reverts to a polynomial; positive nonintegral values for N afford a new range of interpolants.

In the case where  $N \in \{0, 1, 2, \dots, L\}$  the interpolant  $y^*(x)$ , as defined by (2), becomes degenerate in the sense that in either of the intervals x < -A, x > -A, it can be written as a polynomial containing less than L + 2 undetermined coefficients. For such a case, we choose a new non-polynomial interpolant  $y^{**}(x)$ , defined as

$$(4) y^{**}(x) = \sum_{p=0}^{L} a_p x^p + b |A + x|^N \log |A + x|, N \in \{0, 1, 2, \cdots, L\}.$$

If N = 0, the interpolant has a logarithmic singularity at x = -A.

3. The Formulae. A class of two-point explicit formulae is derived after the manner of [1]. The formula to be obtained will predict a value  $y_r$  which approximates to  $y(x_r)$ , the theoretical solution of (1) at  $x = x_r$ . If the solution of (1) is represented in the range  $[x_n, x_{n+1}]$  by the interpolant F(x), the following equations must hold

(5) 
$$F(x_n) = y_n; F(x_{n+1}) = y_{n+1};$$

$$\left[\frac{d^s F(x)}{dx^s}\right]_{x=x_n} = f_n^{(s-1)}, s = 1, 2, \dots, S,$$

where, utilising (1),

$$f_n^{(s)} \equiv \left[\frac{d^s f(x,y)}{dx^s}\right]_{x=x_n,y=y_n} = \left[\frac{\partial f^{(s-1)}(x,y)}{\partial x} + f(x,y) \frac{\partial f^{(s-1)}(x,y)}{\partial y}\right]_{x=x_n,y=y_n}$$

provided all the derivatives concerned exist. The value of S is so chosen that the number of equations in (5), namely S+2, exceeds by unity the number of undetermined coefficients in F(x). The eliminant of these undetermined coefficients from (5) then gives the required algorithm.

If  $F(x) = y^*(x)$ , as defined by (2), then S = L + 1, and the eliminant is found to be

$$(6) y_{n+1} - y_n = \sum_{k=1}^{L} \frac{h^k}{k!} f_n^{(k-1)} + \frac{(A+x_n)^{L+1}}{\alpha_L^N} f_n^{(L)} \left[ \left( 1 + \frac{h}{A+x_n} \right)^N - 1 - \sum_{k=1}^{L} \frac{\alpha_{k-1}^N}{k!} \left( \frac{h}{A+x_n} \right)^k \right],$$

where  $\alpha_r^m \equiv m(m-1) \cdots (m-r)$ , r a non-negative integer.

It should be noted that the expression for  $y^*$  given by (2) is not differentiable at x = -A and this point is necessarily excluded. In practice, this creates no difficulty since, in the case of negative N, integration through the station x = -A, that is, through the singularity of the interpolant would not be contemplated. It will therefore be assumed that formulae of class (6) will be applied entirely in one of the two ranges x < -A, x > -A.

Each formula of class (6) is a truncated Taylor series, with a perturbation

term. Since the expression in square brackets in (6) is the difference between  $(1 + h/(A + x_n))^N$  and the first L + 1 terms of the binomial series for the same expression, it follows that the perturbation term is of order at least  $h^{L+1}$ . In fact, the first term in the expansion of the perturbation term turns out to be  $h^{L+1}f_n^{(L)}/(L+1)!$ , and thus the right-hand side of (6) can be regarded as the first L+2 terms of a Taylor series together with a perturbing term of order  $h^{L+2}$ .

Taylor expansion of (6) gives the following expression for truncation error, defined as

(7) 
$$T.E. = y_{n+1} - y(x_{n+1}),$$

$$T.E. = \sum_{q=1}^{\infty} T_q \frac{h^{L+q+1}}{(L+q+1)!},$$

where

$$T_q = -f_n^{(L+q)} + \frac{\alpha_{q-1}^{N-L-1}}{(A+x_n)^q} f_n^{(L)}.$$

The values of the parameters A and N are now chosen to satisfy  $T_1 = T_2 = 0$ . These values are

(8) 
$$-A_{(n)} = x_n - \frac{f_n^{(L+1)} f_n^{(L)}}{(f_n^{(L+1)})^2 - f_n^{(L)} f_n^{(L+2)}},$$

$$N_{(n)} = L + 1 + \frac{(f_n^{(L+1)})^2}{(f_n^{(L+1)})^2 - f_n^{(L)} f_n^{(L+2)}}.$$

 $A_{(n)}$  and  $N_{(n)}$  are estimates for A and N respectively, based on derivatives of f(x,y) evaluated at  $x=x_n$ ,  $y=y_n$ . The value of L, the degree of the polynomial part of  $y^*$  is at our disposal. A practical upper bound for L is usually dictated by the complication of deducing the higher derivatives of f(x,y) from (1). However, since the principal truncation error of the overall process is now  $T_3h^{L+4}/(L+4)!$ , quite modest values for L give acceptably small truncation errors.

Let us now consider the class of formulae obtained by the above procedure when  $F(x) = y^{**}(x)$ , as defined by (4). This class is found to be

$$(9) y_{n+1} - y_n = \sum_{k=1}^{L} \frac{h^k}{k!} f_n^{(k-1)} + \frac{(-1)^{L-N} (A + x_n)^{L+1} f_n^{(L)}}{N! (L - N)!} \\ \left[ \left( 1 + \frac{h}{A + x_n} \right)^N \log \left( 1 + \frac{h}{A + x_n} \right) - \sum_{k=1}^{L} \left\{ \frac{h^k \alpha_{k-1}^N}{k! (A + x_n)^k} \sum_{j=0}^{k-1} \frac{1}{N - j} \right\} \right],$$

where, once again, the use of a formula of this class to integrate (1) through an interval containing x = -A is precluded. Since  $x_{n+1} = x_n + h$ , this restriction implies that the term  $1 + h/(A + x_n)$ , which appears raised to a possibly fractional power N in (6) and as the argument of a logarithm in (9), cannot be negative. Each formula of class (9) is again a Taylor series with a perturbation term of order  $h^{L+2}$ .

If N takes the value  $\tilde{N}$  where

$$\tilde{N} \in \{0, 1, 2, \cdots, L\},\$$

then the formulae of class (6) are not defined. However if we consider the limit as  $N \to \tilde{N}$ , then the value, in the limit, of the perturbed term in (6) can be calculated

using L'Hôpital's Rule. The resulting formula is identical with (9). The choice of  $y^{**}(x)$ , defined by (4), as the alternative local interpolant in the case when condition (3) is violated, is thus justified. The truncation error series for (9) is that given by (7), when N is replaced by  $\tilde{N}$ . Again, the truncation error of the overall method is of order  $h^{L+4}$ .

Formulae (6) and (9) may also be derived as follows. Consider a change of dependent variable from y to  $\eta$ , where

(11) 
$$\eta = y - b |A + x|^N, \qquad x \neq -A.$$

The initial value problem (1) now becomes

(12) 
$$\eta' = \frac{d\eta}{dx} = g(x,\eta); \qquad \eta(x_0) = \eta_0.$$

Consider the two-point explicit formula for the solution of (12), based on a polynomial interpolant, and with a truncation error one order less than that of the class (6) which is sought. This formula is the truncated Taylor series

(13) 
$$\eta_{n+1} - \eta_n = \sum_{k=1}^L \frac{h^k}{k!} \eta_n^{(k)},$$

where

$$\eta_n^{(k)} \equiv \left[ \frac{d^n \eta(x, \eta)}{dx^n} \right]_{x=x_n, \eta=\eta_n}.$$

The truncation error is

(14) 
$$\text{T.E.} = \sum_{q=1}^{\infty} M_q \frac{h^{L+q}}{(L+q)!},$$

where

$$M_q = \eta_n^{(L+q)}.$$

Solving (12) for  $\eta(x)$  by a two-point explicit formula based on a polynomial interpolant is equivalent to solving (1) for y(x) by a two-point explicit formula based on an interpolant of the type (2). Consequently, we substitute from (11) into (13) to get the formula

$$y_{n+1} - y_n = \beta [(A + x_n + h)^N - (A + x_n)^N] + \sum_{k=1}^L \frac{h^k}{k!} \cdot \{y_n^{(k)} - \beta \alpha_{k-1}^N (A + x_n)^{N-k}\},$$

where

$$\beta = b \quad \text{if} \quad x > -A$$

$$\beta = (-1)^N b \quad \text{if} \quad x < -A.$$

(It will be recalled that the final formula will be used entirely in one of these two ranges.)

Formula (15) still contains the undetermined coefficient  $\beta$ , but if the principal part of the truncation error is set to zero, then, by (14),

$$\eta_n^{(L+1)} = y_n^{(L+1)} - \beta \alpha_L^N (A + x_n)^{N-L-1} = 0,$$

giving a value for  $\beta$ . With this value, and with  $y_n^{(k+1)}$  replaced by  $f_n^{(k)}$ , formula (15) becomes identical with (6). Its truncation error is now

T.E. = 
$$\sum_{q=2}^{\infty} M_q \frac{h^{L+q}}{(L+q)!}$$
,

where it is easily verified that  $M_{q+1} = T_q$ .

Formulae of class (9) can be similarly derived by considering the transformation

$$\eta = y - b | A + x |^{N} \log | A + x |.$$

- 4. Applications. The formulae derived in the last section can be applied in a number of different ways.
- I. If the initial condition  $y(x_0) = y_0$  of (1) is used, equations (8) will yield initial estimates  $A_{(0)}$  and  $N_{(0)}$ . These values are substituted for A and N respectively in equation (6), which is now solved to give  $y_1$ . With this value available, equation (8) affords newer estimates  $A_{(1)}$  and  $N_{(1)}$ , and these are now substituted for A and N in (6), which now yields  $y_2$ . Proceeding in this way, applying (8) and (6) alternately, a numerical solution of (1) is obtained, together with a sequence of estimates  $\{-A_{(n)}\}$  and  $\{N_{(n)}\}$  indicating the position and nature of a possible singularity.

At each step, a test is made to see whether  $N_{(n)} = \tilde{N}$ , where  $\tilde{N} \in \{0, 1, 2, \dots, L\}$ . (In practice, this is assumed to be the case if  $|N_{(n)} - \tilde{N}| < \epsilon$ , where  $\epsilon$  has a small positive pre-assigned value. This device will be referred to as the  $\epsilon$ -switch.) Should  $N_{(n)} = \tilde{N}$ , then the formula of class (6) is replaced by the corresponding formula of class (9).

- If, in (2), the parameters A and N had been regarded as undetermined coefficients and eliminated in the same way as b and  $a_p$  ( $p=0, 1, \dots, L$ ), another class of formulae would have been obtained, which would, under certain circumstances, give a numerical solution of (1) equivalent to that obtained by the process described above. This new class of formulae would, however, be vastly more complicated, and no separate estimate of the position and nature of a singularity could be obtained. The circumstance in which the method would fail would be when the value of  $N_{(n)}$  (no longer explicitly available) came too close to one of the values  $\tilde{N}$ .
- II. The nature of the problem giving rise to the differential equation (1) may be such that values for A and N are known in advance: these values should then be substituted into (6), or (9). If only one of A and N is so known, the other can be estimated by setting  $T_1 = 0$ .
- III. A third technique, which combines I and II appears to give the best results in most cases where no advance knowledge of A or N is available. A solution for (1) is obtained as described in I: this is called the *initial solution*. It is continued up to the station  $x_m$  at which the difference between  $x_m$  and  $-A_{(m)}$  is small (assuming that any possible singularity of the theoretical solution lies to the right of the initial value  $x_0$ ). If the corresponding value of  $N_{(m)}$  is negative or zero (within the tolerance of the  $\epsilon$ -switch) the presence of a singularity at  $-A_{(m)}$  is indicated. The values of  $A_{(m)}$  and  $N_{(m)}$  are then regarded as fixed estimates for A and N, and are substituted into (6) to afford a second solution for y as in II above. This is the improved solution.

It is important to note that, for a given L, the estimates  $A_{(n)}$  and  $N_{(n)}$ , computed from (8) during the initial solution, require evaluation of derivatives of f up to order L+2. When computing the improved solution, the value of L assigned in (6) or (9) should thus be increased by two, in order to preserve the same order of overall truncation error: derivatives of f up to order L+2 will thus be used in the improved solution as well as in the initial solution.

5. Numerical Results. In view of the variety of possible interpolants contained in the general local interpolants (2) and (4), it was felt that fairly extensive numerical testing was essential. Accordingly, numerical solutions, by method III of the last section, are given for three different differential equations. In each case the algorithm has a truncation error of order  $h^5$ ; that is L=1 for the initial solution and L=3 for the improved solution, and derivatives of f up to order three are involved. For comparison, a solution of each problem is given by a standard Runge-Kutta method (the Kutta-Simpson one-third rule) and also by a Taylor series method. The latter is included since it makes use of exactly the same derivatives of f as method III proposed in this paper. In every solution quoted, the truncation error of the algorithm is of order  $h^5$ , and h has the value 0.05 throughout: the  $\epsilon$ -switch is set with  $\epsilon=0.05$ . The calculations were performed on the IBM 1620 computer at the University of St. Andrews, working in floating point to fourteen decimal places.

For each example, the following results are quoted in order.

- (i) Theoretical solution of the differential equation.
- (ii) Initial solution.
- (iii)  $\{N_{(n)}\}\$ , the sequence of estimates for N.
- (iv)  $\{-A_{(n)}\}\$ , the sequence of estimates for -A.
- (v) Improved solution.
- (vi) Solution by Runge-Kutta.
- (vii) Solution by Taylor series, quoted at last tabulated point only. The following examples are considered.

Example 1.  $y' = 1 + y^2$ ; y(0) = 1. Theoretical solution:  $y = \tan(x + \pi/4)$ . Example 2.  $xy' = y + 5x^2e^{y/5x}$ ; y(1) = 0. Theoretical solution:  $y = -5x \log(2 - x)$ .

Example 3.  $(1-x)y'=y\log y$ ;  $y(0)=e^{0.2}$ . Theoretical solution:  $y=e^{0.2/(1-x)}$ . It should be noted that, for the values of L used, none of the theoretical solutions to the above problems is exactly representable by an interpolant of the type (2) or (4).

Results (i)-(vii) are given for Examples 1-3 in Tables 1-3 respectively. In Table 1, it is seen that not only does the method, applied to this example, give a much more accurate solution than do comparable classical methods, but that the estimates for the nature and position of the singularity of the solution (a simple pole at  $x = \pi/4 = 0.785398163$ ) are good.

For Example 2, the improved solution is only a slight improvement on the Runge-Kutta solution. A value near 2 for -A is clearly indicated, and although the sequence  $\{N_{(n)}\}$  does not give as good an indication as it does in Example 1, nevertheless the falling away towards zero of  $N_{(n)}$  as  $x \to -A$  correctly suggests a logarithmic singularity. A smaller value for h in the region where  $\{N_{(n)}\}$  changes rapidly would give a more conclusive indication.

Table 1.  $y' = 1 + y^2$ ; y(0) = 1

x	(i) Theoretical	(ii) Initial Solution	(iii) X	(iv)	() Improved	(v) Improved Solution	(vi) Runge-Kutta	i) Kutta
	noronos:	y y	$I_{\mathbf{V}}(n)$	(u) 	y	Error	y	Error
0	1.000000000	1.000000000	-2.000000000	+1.0000000000	1.000000000	0.000000000	1.000000000	0.000000000
.05	1.105355590	1.105355493	-1.675437652	.920801447	1.105355583	<b>-</b> .000000000 -	1.105355603	.000000012
.10	1.223048880	1.223048668	-1.459538749	.871052433	1.223048865	000000015	1.223048901	000000021
.15	1.356087851	1.356087497	-1.311929388	.839170053	1.356087827	-000000023	1.356087867	.000000015
.20	1.508497647	1.508497114	-1.209581045	.818606761	1.508497613	000000033	1.508497619	-000000027
.25	1.685796417	1.685795650	-1.138345499	.805402497	1.685796372	-000000045	1.685796252	-000000164
.30	1.895765122	1.895764043	-1.089014193	.797042894	1.895765063	-000000029	1.895764601	-000000521
.35	2.149747640	2.149746124	-1.055313510	.791876269	2.149747562	000000078	2.149746231	-000001408
.40	2.464962756	2.464960611	-1.032812028	.788793751	2.464962653	-000000103	2.464959126	-000003930
.45	2.868884028	2.868880924	-1.018291295	.787043022	2.86883887	-000000140	2.868874581	-000009446
.50	3.408223442	3.408218788	-1.009367173	.786114151	3.408223248	-000000197	3.408197466	-000025975
.55	4.169364045	4.169356669	-1.004253830	.785666286	4.169363751	-000000294	4.169284574	-000079471
99.	5.331855223	5.331842457	-1.001612640	.785478455	5.331854741	-000000481	5.331563775	-000291447
.65	7.340436575	7.340410941	-1.000453697	.785415026	7.340435634	-000000040	7.338975331	001461243
2.	11.681373800	11.681304752	-1.000071263	.785400289	11.681370972	-000002828	11.668014352	-0.013359447
.75	28.238252850	28.237817988	-1.000002095	.785398727	28.238208178	-000044671	27.694702600	-.543550249

(vii) Taylor series solution at x = .75: y = 25.710677827; error = -2.527575022.

0 = 0
$\widehat{-}$
y(1
2
$5x^2e^{y/5x}$ ;
-
+
2:
xh'
જાં
TABLE

i) Kutta	Error	0.000000000	-000000246	77,000,000 -	- 000000055	-000001597	-000002074	-000002637	-000003308	-000004115	-0000002092	-000000305	-00000186	-000000299	-000011721	-000013807	-000014164	-000005244	+.000041477	-000723519
(vii) Runge-Kutta	y	0.000000000	269289548	57,9482313	338860119	1.798011355	2.318385060	2.907782045	3.575776058	4.334314139	5.198598756	6.188428343	7.330318068	8.661022927	10.233757115	12.130061851	14.484927047	17.548354615	21.874599860	29.207666148
Solution	Error	0.000000000	.00000018	.00000043	00000000	.00000174	.000000248	.000000345	.000000476	.000000653	968000000	.000001235	.000001716	.000002406	.000003401	.000004779	.000006285	.000005113	-000022224	-000297599
(iv) (iv) Improved Solution	y	0.000000000	0.269289814	0.579482879	0.934485920 1.338861496	1.798013127	2.318387383	2.907785029	3.575779842	4.334318908	5.198604750	6.188435881	7.330327571	8.661034933	10.233772238	12.130080439	14.484947497	17.548364973	21.874536159	29.208092067
(iv)	(u) 17	1.882400000	1.890622634	1.898813240	1.900909320	1.922746768	1.930447107	1.937970244	1.945288719	1.952371535	1.959183613	1.965685156	1.971830878	1.977569089	1.982840589	1.987577322	1.991700730	1.995119690	1.997727729	1.999397110
(iii)	(u) A [	.529400000	.515224966	.500312304	484619100	450643773	.432221428	.412736273	.392097252	.376202699	.346938751	.322177469	.295774595	.267566869	.237368798	.204968740	.170124120	.132555528	.091939196	.047895239
(ii) Initial	y	0.000000000	269289785	.579482845	. 934483880	1.798013077	2.318387333	2.907784986	3.575779820	4.334318933	5.198604871	6.188436191	7.330328263	8.661036416	10.233775454	12.130087799	14.484966151	17.548421303	21.874768973	29.209952281
(i) Theoretical	y	0.000000000	269289795	.579482836	. 934483844	1.798012952	2.318387135	2.907784683	3.575779366	4.334318255	5.198603854	6.188434645	7.330325854	8.661032527	10.233768836	12.130075659	14.484941211	17.548359860	21.874558383	29.208389667
s		1.0	1.05	1.10	1.I5	25.	1.30	1.35	1.40	1.45	1.50	1.55	1.60	1.65	1.70	1.75	1.80	1.85	1.90	1.95

(vii) Taylor series solution at x = 1.95: y = 29.060018867; error = -.148370799.

Table 3.  $(1-x)y'=y\log y$ ;  $y(0)=e^{0.2}$ 

ii) Kutta Error		0.000000000	000000000	000000000	1 00000000	000000002	-000000004	800000000 -	000000015	000000030	000000063	000000143	-000000357	-000001007	000003370	000014292	000085796	000895247	025420629	-7.484338140
(vii) Runge-Kutta	y	1.221402758	1.234327534	1.248848868	1.203280634	1.305605169	1.330712192	1.360282367	1.395612409	1.438550978	1.491824633	1.559623353	1.648720913	1.770793945	1.947730670	2.225526636	2.718196032	3.792772647	7.363635469	47.113811892
.) Solution	Error	0.000000000	.000000036	.00000090	0/100000	.00000468	.000000748	.000001196	.000001936	.000003207	.000005501	168600000	.000018938	.000039417	.000091814	.000250095	.000855710	.004181633	.037961376	1.191160473
(iii) (iv) Improved Solution $A_{\text{Color}}$	y	1.221402758	1.234327572	1.248848959	1.205281025	1.305605640	1.330712946	1.360283572	1.395614361	1.438554217	1.491830199	1.559633389	1.648740209	1.770834369	1.947825855	2.225791024	2.719137539	3.797849528	7.427017475	55.789310506
(iv)	(u) • • •	.920906567	.921759151	.922684194	925091557	.925999876	.927331377	.928806510	.930449825	.932291804	.934379768	.936735577	.939449532	.942596174	.946288174	.950681552	.955999770	.962578476	.970963529	.982194355
	(u)	-1.030619796	-1.033505662	-1.036821902	-1.040059091 -1.045133111	-1.050394217	-1.056640134	-1.064135458	-1.073241063	-1.084459999	-1.098511512	-1.116455105	-1.139908307	-1.171450909	-1.215429777	-1.279712600	-1.380005708	-1.552538406	-1.903674669	-2.967132292
(ii) Initial	h.	1.221402758	1.234327535	1.248848869	1.205280855	1.305605173	1.330712200	1.360282381	1.395612435	1.438551028	1.491824736	1.559623580	1.648721463	1.770795458	1.947735587	2.225546784	2.718312279	3.793933715	7.395357859	57.118901360
(i) Theoretical	y y	1.221402758	1.234327535	1.248848869	1.205280855	1.305605172	1.330712197	1.360282376	1.395612425	1.438551009	1.491824697	1.559623497	1.648721270	1.770794952	1.947734041	2.225540928	2.718281828	3.793667894	7.389056098	54.598150033
8		0	.05	.10	06.	25.	.30	.35	.40	.45	.50	.55	09:	.65	.70	.75	08:	.85	06:	.95

(vii) Taylor series solution at x = .95: y = 32.512834270; error = -22.085315762.

Example 3 is perhaps the most testing, since the theoretical solution contains an essential singularity at x = 1. This is suggested by the steep increase in the magnitude of  $N_{(n)}$  as  $x_n \to -A_{(n)}$ . Despite the fact that the improved solution is computed by setting N=-2.967132292 (a poor estimate for  $-\infty$ ), the final solution is reasonably good for such a difficult equation. Again, the sequences  $\{N_{(n)}\}$ ,  $\{-A_{(n)}\}$  suggest that a smaller value for h be used as  $x_n \to -A_{(n)}$ .

In each case, the solution by Taylor series is poorer than that by Runge-Kutta.

**6.** Generalizations. Consideration of the second method of derivation given in Section 3 shows that implicit formulae and multistep formulae could be derived along the lines of (6) and (9). Indeed, any of the formulae listed by Lambert and Mitchell [4] have their counterpart. However, there is a good practical reason for preferring the two-point explicit class.

Every formula of the class considered in [4] has a truncation error of the same form as (14). It follows that formulae (8) for  $N_{(n)}$  and  $-A_{(n)}$  will have the same form for every generalization of (6) and (9) corresponding to the formulae of [4]. However, it is only for the two-point explicit class considered in this paper that the order of the derivatives of f, needed to evaluate  $N_{(n)}$  and  $-A_{(n)}$ , follow consecutively upon the order of the derivatives of f used in the main formulae (6) or (9). For implicit and multistep formulae there is a "gap". Thus, for example, the counterpart of Simpson's Rule will involve no derivatives of f in the main formula, but since Simpson's Rule has a truncation error of order  $h^5$ , then  $f^{(4)}$  and  $f^{(5)}$  will appear in the formulae for  $N_{(n)}$  and  $-A_{(n)}$ . Increased accuracy of a finite difference formula for the solution of (1) can be achieved either by increasing the number of points in the formula, or by increasing the order of the derivatives of f involved. The former course, with its attendant difficulties over starting values and possible instability, can only be successfully argued if the labour involved in calculating and evaluating higher derivatives of f is unacceptable. Since this calculation must in any case be done in order to evaluate  $N_{(n)}$  and  $-A_{(n)}$ , the case for implicit and multistep generalizations of (6) and (9) would appear to be a weak one.

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