NUMERICAL INTEGRATION OF NONLINEAR DIFFERENTIAL EQUATIONS BY USE OF RATIONAL APPROXIMATION

FINAL REPORT
15 January 1965 - 14 July 1967

Task Order Contract No. NASr-63(07)
NASA Hq. R&D 80X0108(64)

MRI Project No. 2760-P

For

Office of Grants and Research Contracts
Code SC
National Aeronautics and Space Administration
Washington, D. C. 20546

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425 VOLKER BOULEVARD/KANSAS CITY, MISSOURI 64110/AC 816 LO 1-0202

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by

Yudell L. Luke
Wyman Fair
Jet Wimp

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PREFACE

This report covers research initiated by Headquarters, National Aeronautics and Space Administration on Contract NASA Hq. R&D 80X0108(64), 10-74-740-124-08-06-11, PR10-2487. "Nonlinear Dynamics of Thin Shell Structures." The research work upon which this report is based was accomplished at Midwest Research Institute with Mr. Howard Wolko as project monitor.

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Approved for:

MIDWEST RESEARCH INSTITUTE

S L Levy

Sheldon L. Levy, Director
Mathematics and Physics Division

14 July 1967

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I. SUMMARY AND INTRODUCTION

In the numerical treatment of ordinary linear differential equations there are many effective integration formulas which yield quick, reliable results. These techniques depend heavily on the fact that solutions to linear differential equations are very well behaved in that all the needed higher order derivatives exist in the range of interest.

In general, the theory of ordinary nonlinear differential equations offers no clue as to the singularities of the solutions of such equations. Thus the detection of singularities must be accomplished heuristically. Obviously the usual numerical integration techniques fail in the region of such singularities. Not only are the results inaccurate near a singularity, but also the location of such a point evades detection. Hence, new techniques must be developed which will deal effectively with the problem of singularities of solutions to nonlinear differential equations.

Recently we obtained an algorithum for computing rational approximations to the solution of a wide class of nonlinear differential equations, see [1]. Although this technique cannot be extended to arbitrary nonlinear equations, it clearly demonstrates the power of rational approximations in dealing with a function which has singular points in the range of interest. These approximations ascertain the existence of zeros and poles of a function and locate these critical points with great accuracy. Rational approximations also allow accurate computation of the function near a singular point -- a decided advantage over the usual approximations.

In light of the advantages cited above, it is desirable to obtain formulas for numerical integration of ordinary nonlinear differential equations which are based on rational approximations.

In Section II we develop multi-step predictor and corrector formulas for numerical integration. In Section III we obtain the truncation errors associated with such formulas. The results are applied to some examples in Section IV. A recommended procedure for the use of these rational approximations in the numerical treatment of nonlinear differential equations is outlined in Section V.

II. DEVELOPMENT OF INTEGRATION FORMULAS

Here we develop multi-step predictor and corrector formulas based on rational functions for the numerical integration of the differential equation

$$y' = f(x,y) \ , \ y(x_o) = y_o \quad . \tag{2.1}$$

The extension of the formulas to higher order equations is immediate.

It is assumed that all the needed starting values are available. We wish to approximate the solution to (2.1) by a rational function. We write

$$y(x) = \frac{P_m(x)}{Q_n(x)} + E_{m,n}(x) \ ,$$

$$P_m(x) = \sum_{j=o}^{m} a_j x^j \text{ and } Q_n(x) = 1 + \sum_{j=1}^{m} b_j x^j \ , \tag{2.2}$$

where the coefficients a_j and b_j are unknown.

In order to obtain a k-step method, it is sufficient to require that either $n+m = 2k$, or $n+m = 2k-1$. For convenience, we set

$$L_{m,n}(x) = Q_n(x)y(x) - P_m(x) \ , \tag{2.3}$$

$$L_{m,n}'(x) = Q_n'(x)y(x) + Q_n(x)y'(x) - P_m'(x) \ , \tag{2.4}$$

and $y(x_j) = y_j$ for a set of equally spaced interpolation points $x_o<x_1<\ldots<x_{k+1}$. Without loss of generality, $x_o = 0$ and $x_{j+1} = x_j+1$. We develop the predictor and corrector formulas for the case $m+n = 2k$ and then indicate the necessary changes for the case $m+n = 2k-1$.

Let $m+n = 2k$ and require that in (2.3) - (2.4),

$$L_{m,n}(x_j) = 0 \qquad j = 0,1,\ldots, k+1 ,$$

$$L_{m,n}'(x_j) = 0 \qquad j = 1,2,\ldots, k . \tag{2.5}$$

The resulting system of equations in the unknowns a_j and b_j has a solution, if and only if, the following determinant vanishes;

$$\Delta_p = \begin{vmatrix} R_{k+1,m+1} & S_{k+1,n+1} \\ & \\ T_{k,m+1} & U_{k,n+1} \end{vmatrix} = 0 , \tag{2.6}$$

where the entries in the determinant are rectangular arrays of the size indicated by the subscripts, and if h_{ij} denotes the $i,j\underline{th}$ entry in a rectangular array $H_{p,j}$, the arrays in the determinant (2.6) are defined by

$$r_{ij} = (i-1)^{j-1},\ i = 1,2,\ldots,k+2 \ ;\ j = 1,2,\ldots,m+1 \text{ and } r_{11}=1 ,$$

$$s_{ij} = (i-1)^{j-1}y_{i-1},\ i = 1,2,\ldots,k+2 \ ;\ j = 1,2,\ldots,n+1 \text{ and } s_{11}=y_o ,$$

$$t_{ij} = (j-1)(i)^{j-2},\ i = 1,2,\ldots,k \ ;\ j = 1,2,\ldots,m+1 , \tag{2.7}$$

$$u_{ij} = (j-1)(i)^{j-2}y_i+(i)^{j-1}y_i',\ i = 1,2,\ldots,k \ ;\ j = 1,2,\ldots,n+1 .$$

We call Δ_p the predictor determinant. To obtain the corrector determinant, Δ_c, corresponding to the conditions (2.5), replace the first row of (2.6) by the last row of (2.6) with k replaced by $k+1$. After setting $\Delta_p = \Delta_c = 0$ and expanding the determinants, we obtain

$$\Delta_p = Ay_{k+1}+B = 0 , \tag{2.7}$$

$$\Delta_c = Cy^2_{k+1}+Dy_{k+1}+E = 0 , \tag{2.8}$$

where the coefficients in (2.7) depend on y_j and y'_j , $j = 0,1,\ldots,k$, and the coefficients in (2.8) depend not only on these values, but also on y'_{k+1} . Note that (2.8) requires solutions of a quadratic equation for the corrected value. This is discussed in more detail later. Thus after setting $y(x) = y(x_o+hx)$ we obtain the final form for the predicted and corrected values at y_{k+1} by solving (2.7) and (2.8). The predicted value of y_{k+1} is obtained from (2.7), the differential equation is employed to get a predicted y'_{k+1} and the corrector is used repeatedly until the results stabilize. However, for small h , the predictor can be used alone.

For the case $m+n = 2k-1$, we get the predictor from (2.6) by deleting the first row and we get the corrector from this result by increasing the row indices of the last k rows by unity. In illustration, three cases are listed below.

If $m=n=1$:

$$y_2(\text{predicted}) = \frac{2y_o y_1 - 2y_1^2 + hy_o y_1'}{2y_o - 2y_1 + hy_1'} ,$$

and the corresponding corrector formula is

$$y_2^2 - 2y_1 y_2 + (y_1^2 - hy_1' y_2') = 0 .$$

For $m=1$, $n=2$:

$$y_2(\text{predicted}) = \frac{y_o^2(3y_1+hy_1') + y_1^2(2hy_o'-3y_o)}{y_o(4y_o-5y_1+hy_1') + y_1(y_1+2hy_o')-2h^2 y_o' y_1'} ,$$

and for the corrector, the values in (2.8) are given by

$$C = 3y_1 - 4y_o - y_1'$$

$$D = 5y_o y_1 - 3y_1^2 + y_o y_1'$$

$$E = 2y_o' y_2'(y_1'+y_1) - y_1^2(y_o+2y_2') .$$

For m=n=2 :

$$y_3(\text{predicted}) = \frac{(2hy_o'-3y_o)d_1 + y_1d_2 + y_2d_3}{-3d_1 + d_2 + d_3} ,$$

where

$$d_1 = (y_1-y_2)^2 - h^2y_1'y_2' ,$$

$$d_2 = \frac{1}{2} (4y_o-3hy_o'-4y_2)(y_1-y_2) - \frac{1}{2} hy_2'(5y_1-5y_o+6hy_o') ,$$

$$d_3 = hy_1'(4y_o-3hy_o'-4y_2) - (y_1-y_2)(5y_1-5y_o+6hy_o') ,$$

and for the corrector, the values in (2.8) are

$$C = y_1-y_o-hy_o'-\frac{1}{4} hy_1' ,$$

$$D = 2hy_o'y_1+y_o^2-y_1^2+y_1-y_o+\frac{1}{2} hy_oy_1' ,$$

$$E = y_oy_1^2-y_o^2y_1-hy_o'y_1^2-hy_2'(y_1-y_o)^2 - \frac{1}{4} hy_o^2y_1'+h^3y_o'y_1'y_2' .$$

III. TRUNCATION ERROR

In this section we develop an expression for the truncation error associated with the integration formulas of Section II. We restrict ourselves to the predictor formula for the case $m+n = 2k$ (see (2.5) - (2.7)). The other cases are handled similarly and, since we are interested only in the order of the truncation error, the treatment of one case is sufficient.

As in (2.2), we set

$$y(x) = \frac{P_m(x)}{Q_n(x)} + E_{m,n}(x) . \tag{3.1}$$

Let $x_o<x<\ldots<x_{k+1}$ be equally spaced interpolation points and assume y is $(2k+1)$ times differentiable in the interval $[x_o,x_{k+1}]$ except at the poles $C_1,C_2,\ldots,C_v$ of orders $s_1,s_2,\ldots,s_v$ respectively. Thus, if

$$r(x) = \prod_{j=1}^{v} (x-C_j)^{s_j} \quad , \tag{3.2}$$

Then $r(x)y(x)$ is $(2k+1)$ times differentiable in $[x_o, x_{k+1}]$. Now we set

$$E_{m,n}(x) = \frac{\pi_{m,n}(x)F(x)}{Q_n(x)r(x)} \quad ,$$

where (3.3)

$$\pi_{m,n}(x) = \prod_{j=1}^{k} (x-x_j)^2 \quad ,$$

and $F(x)$ is a function to be determined. Now if

$$L_{m,n}(x) = y(x)Q_n(x) - P_m(x) \quad , \tag{3.4}$$

then for the case $m+n = 2k$, the predictor formula requires

$$\begin{aligned} L_{m,n}(x_i) &= 0 \quad , \quad i = 0,1,\ldots,k+1 \quad , \\ L_{m,n}'(x_i) &= 0 \quad , \quad i = 1,2,\ldots,k \quad . \end{aligned} \tag{3.5}$$

Consider the function

$$g(t) = r(t)L_{m,n}(t)\,\frac{(t-c)}{(x-c)} - F(x)\pi_{m,n}(t)\,\frac{(t-d)}{(x-d)} \quad . \tag{3.6}$$

We have

$$g(x_i) = 0 = g'(x_i) \quad , \quad i = 1,2,\ldots,k \quad . \tag{3.7}$$

Now c and d in (3.6) can be determined so that $g'(x_o) = 0$. Thus, $g''(t)$ has $2k$ zeros in the interval $[x_o, x_{k+1}]$. Repeated use of Rolle's theorem guarantees the existence of a number u in the interval $x_o<u<x_{k+1}$ such that $g^{(2k+1)}(u) = 0$. Differentiation of (3.6) (2k+1) times yields

$$0 = \frac{1}{x-c} \frac{d^{2k+1}}{du^{2k+1}} \left\{ r(u)Q_n(u)y(u)(u-c) \right\} - F(x) \frac{(2n+1)!}{x-d} \quad , \qquad (3.8)$$

$$x_o<u<x_{k+1} \quad .$$

Solving for $F(x)$, we get

$$F(x) = \frac{(x-d)}{(x-c)(2k+1)!} \frac{d^{2k+1}}{du^{2k+1}} \left\{ r(u)Q_n(u)y(u)(u-c) \right\} \quad , \qquad (3.9)$$

so that

$$E_{m,n}(x) = \frac{\pi_{m,n}(x)(x-d)}{Q_n(x)r(x)(x-c)(2k+1)!} \frac{d^{2k+1}}{du^{2k+1}} \left\{ r(u)Q_n(u)y(u)(u-c) \right\} \quad . \qquad (3.10)$$

Using the fact that $x_j = X_o + jh$, setting $x = x_{k+1}$ and simplifying, we have

$$E_{m,n}(x) = h^{2k} \frac{(x_{k+1}-d)(k!)^2}{Q_n(x_{k+1})r(x_{k+1})(x_{k+1}-c)(2k+1)!} \frac{d^{2k+1}}{du^{2k+1}} \left\{ r(u)Q_n(u)y(u)(u-c) \right\} . \qquad (3.11)$$

Thus, the order of the truncation error is h^{2k} . The order for the corrector is the same. It is very important to point out that the usual linear k-step integration methods have truncation error of at most order of h^{k+2} , see [2]. Thus, the predictor (2.7) is more accurate than the usual k-step method.

For the case $n+m = 2k-1$, it can be shown as above that the predictor and corrector both have truncation errors of order h^{2k}. Thus for computational purposes, it seems desirable to utilize the approximations (2.6) in which $n+m = 2k-1$.

IV. EXAMPLES AND APPLICATIONS

We apply the results of Section II to three examples. In the first two examples, first order differential equations are treated. Here the approximations (2.7)-(2.8) with $m=1$ and $n=2$ are employed. In the third example, a second order differential equation, we use $m=n=2$. In both cases, the corrector is used repeatedly until successive iterates agree to eight decimal places. The root of (2.8) was chosen which agreed best with the previously computed value of y_{k+1}.

Let $u = \tan(x+\pi/4)$, $v = J_1(x)/J_0(x)$ and let Z be Painlevé's second transcendent. These functions satisfy

$$u' = 1+u^2 \ , \ u(0) = 1 \ , \tag{4.1}$$

$$v' = 1+v^2 - \frac{1}{x} v \ , \ v(0) = 0 \ , \tag{4.2}$$

and

$$Z'' = 2Z^3+xZ+1 \ , \ Z(0) = 1 \ , \ Z'(0) = 0 \ . \tag{4.3}$$

Now u, v and Z have simple poles at $\pi/4$, 2.40482 and 1.1577, respectively. See Tables I, II and III for the results of numerical integration. Notice, that the relative error has a slow rate of growth and that these approximations do indeed detect the presence of a pole in each case. To illustrate this last remark, we have listed in Table II the approximations to the smallest pole of $\tan(x+\pi/4)$ based on use of the predictor only. Here the function was approximated by a linear over a quadratic, and the zeros of the denominator were computed. We point out that this table also indicates that the pole can be computed very accurately if the functional values are known relatively close to the pole.

In Tables I, III and IV, the corrected value that appears is the final result of correcting repeatedly until successive corrected values agreed to eight decimals. For the step size $h = 0.01$, all the intermediate values were computed but these are omitted for the sake of brevity. Note that the computed values beyond the pole are very accurate. Even though this practice of integrating over a pole is not recommended, it does give valuable information about the behavior of the function.

TABLE I

NUMERICAL SOLUTION OF $u' = 1+u^2$, $u(0) = 1$

$u = \tan(x+\pi/4)$

		h = 0.05		h = 0.01	
x	True (u)	Predicted	Corrected	Predicted	Corrected
0.1	1.22305	1.22304	1.22305	1.22305	1.22305
0.2	1.50850	1.50848	1.50850	1.50850	1.50850
0.3	1.89577	1.89574	1.89577	1.89577	1.89577
0.4	2.46496	2.46493	2.46498	2.46496	2.46496
0.5	3.40822	3.40815	3.40826	3.40822	3.40822
0.6	5.33186	5.33165	5.33195	5.33186	5.33186
0.7	11.68137	11.67998	11.68153	11.68138	11.68139
0.8	-68.47967	-68.59667	-68.66273	-68.48685	-68.49443
0.9	- 8.68763	- 8.73393	- 8.68629	- 8.69860	- 8.69493
1.0	- 4.58804	- 4.62137	- 4.64804	- 4.56120	- 4.56121

TABLE II

LOCATION OF POLE OF $\tan(x+\pi/4)$; TRUE POLE; $\pi/4 = 0.785398$

	h = 0.05		h = 0.01
x	Root of $Q_2(x)$	x	Root of $Q_2(x)$
0.60	0.7868	0.76	0.78540 35
0.65	0.7855	0.77	0.78539 82
0.70	0.7869	0.78	0.78540 08
0.75	0.7851	0.79	0.78539 89
0.80	0.7851	0.80	0.78539 65

TABLE III

NUMERICAL SOLUTION OF $v' = 1+v^2 - \frac{1}{x} v, v(0) = 0$

$v = J_1(x)/J_o(x)$

x	True (v)	h = 0.05 Predicted	h = 0.05 Corrected	h = 0.01 Predicted	h = 0.01 Corrected
0.2	0.10050	0.10050	0.10050	0.10050	0.10050
0.4	0.20411	0.20411	0.20411	0.20411	0.20411
0.6	0.31436	0.31436	0.31436	0.31436	0.31436
0.8	0.43584	0.43584	0.43584	0.43584	0.43584
1.0	0.57508	0.57508	0.57508	0.57508	0.57508
1.2	0.74246	0.74246	0.74246	0.74246	0.74246
1.4	0.95606	0.95606	0.95606	0.95606	0.95606
1.6	1.25141	1.25141	1.25142	1.25141	1.25141
1.8	1.71041	1.71041	1.71043	1.71041	1.71041
2.0	2.57592	2.57589	2.57596	2.57592	2.57592
2.2	5.03762	5.03636	5.03698	5.03754	5.03754
2.4	207.43659	126.95138	128.87352	207.31622	207.31021
2.5	-10.27398	-11.13360	-11.64502	-10.28250	-10.28618

TABLE IV

NUMERICAL SOLUTION $Z'' = 2Z^3+xZ+1, Z(0) = 1, Z'(o) = 0$

Z IS PAINLEVE'S SECOND TRANSCENDENT

x	True (Z)	h - 0.05 Predicted	h - 0.05 Corrected	h = 0.01 Predicted	h = 0.01 Corrected
0.2	1.06261	1.06271	1.06267	1.06261	1.06261
0.3	1.14638	1.14634	1.14640	1.14637	1.14638
0.4	1.27415	1.27377	1.27379	1.27415	1.27415
0.5	1.45921	1.45751	1.45730	1.45921	1.45921
0.6	1.72538	1.72170	1.72159	1.72537	1.72538
0.7	2.11844	2.11211	2.11185	2.11840	2.11845
0.8	2.73694	2.72608	2.72581	2.73710	2.73710
0.9	3.83440	3.81512	3.81417	3.83522	3.83520
1.0	6.31100	6.24525	6.25787	6.31763	6.31758
1.1	17.31546	19.30070	21.69210	17.37845	17.38471
1.2	-23.64085	1.62902	-3.06227	*	

* This value could not be computed due to overflow on the computer. The last value computed was for x = 1.14.

V. CONCLUSIONS

It is evident that the integration techniques developed here can be extremely useful, particularly in locating singularities of solutions to nonlinear differential equations and in computing functional values near such points. Before these approximations can be used on a wide scale, several problems must be analyzed. First there is the problem of selecting the correct root of the quadratic equation (2.8) associated with the corrector. Another pertinent question is the stability of the process. This is particularly important when the predictor is used without the corrector. Finally, there is the problem of obtaining stepwise a priori estimates of the error involved in the integration. In connection with the latter, it appears that the predicted value and the first corrected value can be used to estimate the error in much the same way as is done for the usual numerical integration schemes. In the present instance the process is much more complicated for at each stage one must compute the coefficients in the denominator polynomial of the rational approximation and other quantities as evidenced by (3.11). All these questions are interrelated and we recommend further research on these topics.

Our experience to date with the developments in this report suggests that the approximations be employed in the following fashion. The usual integration formulas should be used as long as the solution to a given differential equation is well behaved. If large differences in successive computed values occur (indicative of a pole), employ the rational approximations to locate the pole p. Then introduce a reciprocal transformation in the differential equation to obtain the equation whose solution has a zero at p. In the neighborhood of this zero, the usual integration techniques can be utilized. After having gone a sufficient distance beyond this zero, use the reciprocal transformation to recover the original equation and proceed with the integration.

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