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Full Length Research Paper

A quadratic based integration scheme for the solution of singulo-stiff differential equations

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In this term paper, we designed a quadratic based integration scheme for the solution of initial value problem (IVPs) in ordinary differential equation (ODEs). This was achieved by considering the rational interpolating operator

$$y(x) = \frac{P_m(x)}{1 + q_1 x + q_2 x^2} \approx u(x), \quad \textbf{satisfying } u(x_{n+i}) = y_{n+i}, \qquad i = 0, 1, 2..........$$

A class of rational integrator formula given by

$$y_{n+1} = \sum_{i=0}^{k-1} p_i\, x_{n+1}^i \,/\, 1 + \sum_{i=1}^{KY} p_i x_{n+1}^i$$

in Aashikpelokhai (1991) with K=14 was also implemented and the results compared.
The vector q= (q_1, q2………q_k) are obtained from the simultaneous linear equation (SLE) Sq=b where

$$S_{ij} = \frac{h^{2k-i-j} y_n^{(2k-i-j)}}{(2k-i-j)!\, x_{n+i}^{2k-i-j}}$$

$$b_i = -\frac{h^{2k-i} y_n^{(2k-i)}}{(2k-i)!\, x_{n+1}^{2k-i}}$$

$$\mathbf{P_0 = y_n,}\quad p_j = \sum_{i=1}^{j} \frac{h^{j+1-i} y_n^{(j+1-i)}}{(j+1-i)!\, n_{n+1}^{j+1-i}} + y_n q_{i,} \qquad j = 1(1)3$$

The results as analyzed with the computer show that the integrator copes favourably well with singular problems, stiff problem and singulo-stiff problems.

Keywords: Rational integrators, region of absolute stability, integration scheme, consistency, convergence, stiff and singular problems.

INTRODUCTION

The development of numerical methods for stiff or singular system of ODEs has been attracting much attention in recent times due to their needs in the solution of problem arising from the mathematical formulation of physical situation in chemical kinetics, population models, mechanical oscillation, process control and electrical circuit theory which often leads to initial value problem

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(IVPs) in Ordinary Differential Equation that are singular or stiff or oscillatory. They are mainly from reaction or chemical kinetics see Nunn and Huang (2005)), Lambert (2000), Corles (2001), Norelli (1985), (Willoughy, 1974) and Fatunla (1980, 1982).

The problem for this research paper is to find a numerical solution the I.V.P

$$y^{I} = f(x, y), y(x_0) = y_0, a \le x \le b \qquad (1.1)$$

Where $f(x, y)$ is defined and continued in a region D C [a,b] that are either stiff, singular or oscillatory.

The representation (1.1) does not indicate the nature of the solution function. This suggests that our design of the needed numerical integration must seek to ensure that the integrator we design must be based on functional approximations that have the requisite features.

For a given amount of computation, rational approximation leads to smaller maximum errors than polynomial approximation for the functions most commonly approximated on digital computers. See Ralston A and Rabinowitz (1987).

Rational function has the advantage of automatically picking up the singularities of a given function to the zeros of the denomination. The need to have integrator that can effectively cope well with both singular, stiff or both is enough reason for the search for new integration schemes or formulas which this paper seems to address.

Our aim in this research paper is therefore to solve the problem represented by (1.1) where $f(x, y)$ must satisfy a Lipschitz condition WRT y. In satisfying this desire we must set the following objectives.

- Construction of a rational integrator with a quadratic denominator having one of its members L-state to cope with stiff, singular and oscillation problem
- Determining the performance, stability, characters, consistence and nature of the integrator.
- Development of a Fortran 77 package for the implementation of the integration develop as well as comparing their performance with some established results as seen in section (5.0).

If y(x) is a solution to the problem stated in (1.1) above, the rational function

$$p_n(x) / Q_n(n) = y(x) \qquad (1.2)$$

takes the singularity of the function to be approximated. The singularities of (1.2) are specified by the zeros of $Q_n(x)$. The location of a singularity is not necessary known before hand but it can be recognized by a change in the signs of the denominator [Fatunla, 1986, 1988; Lambert, 1973, 2000). The solution of the IVP in (1.1) may be assumed in some cases to singularities and continuous derivations to the order desired. In such situation it seems very challenging since we do not know enough on the nature and location of the singular points of the ODEs. More so is the glaring fact that the conventional integration methods such as LMM and RKM fail poorly in the neighborhood of the singular points. This may not be too surprising since the algorithm are designed on the basis that the IVP satisfies the existence and uniqueness theorem, so that polynomial interpolation can be successful.

The existing algorithm designed for singular IVPs amongst others are:

- Perturbed polynomials due to: Lambert and Shaw (1996), Shaw (1967) and Lambert (1974).
- Rational methods: Lambert and Shaw (1965), Luke et al. (1975), Niekerk (1987),
- Fatunla (1986, 1998, 1994), and Ikhile (2002).
- Extrapolation process: Fatunla (1986), Ikhile (2001).

Switching function techniques due to Evans and Fatunla (1975), Halin (1976), (1983), Gear and Osterly (1984) and Aashikpelokhai (2000).

Some of the existing methods for stiff integration schemes are: LMM, Exponential Based methods (EBM) and Rational Interpolant based methods.(EBM) and Rational Interpolant based methods.

Aashikelokhai (1991, 1997), Enryte and Pryce (1978), Lambert and Shaw (1965), Lambert (1973), Fatunla (1976, 1978), Dahlquist (1956) suggested different methods of amending the performance of numerical integration formulae which are designed for solving stiff IVPs.

One major conclusion to be drawn from the above discussion is that there is the dire need to have a method that can cope effectively well with different classes of IVPs. In order to successfully carry out the set objective we stated earlier in the research we shall be concerned with the design and analysis of a quadratic based numerical integrator in the next section.

The new integrators

Let R our region of operator be the usual real line. Let UC C^{m+3}(R) be a real operation defined by the identity

$$U(x)[1 + q_1 x + q_2 x^2] \equiv \sum_{r=0}^{m} p_r x^r = p_m(x) \qquad (2.1)$$

and satisfying the constraints

$$u(x_{n+1}) = \{ {}^{y(x_{n+i})\, fori=o}_{y_{n+i}\, fori=0,1} \qquad (2.2)$$

where the function $y \in C^{m+3}(R)$ in what we seek. To where the function $y \in C^{m+3}(R)$ in what we seek. To achieve this we let the Taylor series of U be given by

$$U(x) \equiv \sum_{r=0}^{m+3} C_r x^r \qquad (2.3)$$

while that of y is given by

$$y_{n+1} = \sum_{r=0}^{m+3} \frac{h^r y_n^{(r)}}{r!} \tag{2.4}$$

where

$$\sum_{r=0}^{m+3} C_r x_{n+1}^r \equiv \sum_{r=0}^{m+3} \frac{h^r y_n^{(r)}}{r!}$$

leads us to

$$C_r = \frac{h^r y_n^{(r)}}{r! x_{n+1}^r}, r = 0(1)m+3 \tag{2.5}$$

The given identity (2.1) together with constraints (2.2) gives rise to the parameter evaluation equation (2.6)- (2.9).

$$\begin{pmatrix} c_{m+1} & c_m \\ c_m & c_{m-1} \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = -\begin{pmatrix} c_{m+2} \\ c_{m+1} \end{pmatrix} \tag{2.6}$$

$$p_0 = c_0 = y_n \tag{2.7}$$

$$p_1 = c_1 = c_0 q_1 \tag{2.8}$$

$$p_r = c_r + c_{r-1} q_1 + c_{r-2} q_2 \quad r = 2(1)m \tag{2.9}$$

Employing the parameter evaluation equation along with relation (2.5), we obtain

$$q_1 x_{n+1} = \psi_1(h; y_n^{(m)}) \psi_0^{-1}(h; y_n^{(m)}) \tag{2.10}$$

$$q_2 x_{n+1}^2 = \psi_2(h; y_n^{(m)}) \psi_0^{-1}(h; y_n^{(m)}) \tag{2.11}$$

$$p_1 x_{n+1} = h y_n^{(1)} + y_n \psi_1(h; y_n^{(m)}) \psi_0^{-1}(h; y_n^{(m)}) \tag{2.12}$$

$$p_r x_{n+1}^r = \frac{h^r y_n^{(r)}}{r!} + \frac{h^{r-1} y_n^{(r-1)}}{(r-1)!} \psi_1(h; y_n^{(m)}) \psi_0^{-1}(h; y_n^{(m)}) + \frac{h^{r-2} y_n^{(r-2)}}{(r-2)!} \psi_2(h; y_n^{(m)}) \psi_0^{-1}(h; y_n^{(m)}) \tag{2.13}$$

resulting in the set of integrators

$$y_{n+1} = \left[\sum_{i=0}^{2} \sum_{r=i+1}^{m} \frac{h^{r-1} y_n^{(r-1)}}{(r-1)!} \psi_i(h; y_n^{(m)}) \right] \left[\sum_{i=0}^{2} \psi_i(h; y_n^{(m)}) \right]^{-1} \tag{2.14}$$

where m = 0, 1, 2,…………………

$$\psi_i(h; y_n^{(m)}) = h^i \beta_i(h; y_n^{(m)}), i = 0,1,2.................. \tag{2.15}$$

$$\beta_0(h; y_n^{(m)}) = \left[y_n^{(0)} y_n^{(m+1)} \right] \left[(m-1)!(m+1)! \right]^{-1} - \left[y_n^{(m)} (m!)^{-1} \right]^2 \tag{2.16}$$

$$\beta_1(h; y_n^{(m)}) = \left[y_n^{(m)} y_n^{(m+1)} \right] \left[m!(m+1)! \right]^{-1} - \left[y_n^{(m-1)} y_n^{(m+2)}) \right] \left[(m-1)!(m+1)! \right] \tag{2.17}$$

$$\beta_2(h; y_n^{(m)}) = \left[y_n^{(m)} y_n^{(m+2)} \right] \left[m!(m+2)! \right]^{-1} - \left[y_n^{(m+1)} (m+1)^{-1} \right]^2 \tag{2.18}$$

In the usual form for putting down one-step integrators, the form in (2.14) becomes

$$y_{n+1} = y_n + \left[\sum_{i=0}^{2} \sum_{r=i+1}^{m} \frac{h^{r-1} y_n^{(r-1)}}{(r-1)!} \psi_i(h; y_n^{(m)}) \right] \left[\sum_{i=0}^{2} \psi_i(h; y_n^{(m)}) \right]^{-1} \tag{2.19}$$

Consistency and convergence

It is a common knowledge among derivators of one step integrators that any one-step integrator is convergent and if and only if the one-step integrator is consistent (Lambert, 1976). It is also a common knowledge among this class of researchers that a one-step integrator is consistent if the potential function which is the expression of the integrator representing $\left[y_{n+1} - y_n \right] h^{-1}$, tends to $y_n^{(1)}$ in the limit $h \longrightarrow 0.$ consequently we go about the investigation of the nature of convergence and consistency of our integrators here using the above mentioned properties.

Theorem [Convergence]

The quadratic denominator-based integrators derived above are convergent.

Proof

Re-arranging the normal form of the integrators given by result (2.19) we get:

$$y_{n+1} - y_n = \left[h y_n^{(1)} \left\{ \sum_{i=0}^{2} \psi_i(h; y_n^{(m)}) \right\} + \sum_{i=0}^{m} \frac{h^{r-i} y^{(r-i)}}{(r-i)!} \sum_{i=0}^{2} \psi_i(h; y_n^{(m)}) \right] \left[\sum_{i=0}^{2} \psi_i(h; y_n^{(m)} \right]^{-1}$$

$$= h y_n^{(1)} + \left[\sum_{r=i+2}^{m} \frac{h^{r-i} y_n^{(r-i)}}{(r-i)!} \sum_{i=0}^{2} \psi_i(h; y_n^{(m)}) \right] \left[\sum_{i=0}^{2} \psi_i(h; y_n^{(m)}) \right]^{-1}$$

Hence we write

$$y_{n+1} = y_n + h\phi(h; x_n, y_n)$$

where

$$\phi(h,x_n,y_n)=y_n^{(1)}+\left[\sum_{i=0}^{2}\sum_{r=i+2}^{m}\frac{h^{r-i-1}y_n^{(r-i)}}{(r-i)!}\psi_i(h,y_n^{(m)})\right]\left[\sum_{i=0}^{2}\psi_i(h,y_n^{(m)})\right]^{-1}\longrightarrow y_n^{(1)}$$

in limit as $h\longrightarrow o;$

meaning the integrators are consistent. But they are one-step methods. Hence the integrators are convergent.

STABILITY CONSIDERATIONS

Theorem (Stability function)

The stability function of the Quadratic-based denominator given by

$$s(\bar{h})=\frac{(m+1)(m+2)\sum_{r=0}^{m}\frac{\bar{h}^r}{r!}-2(m+1)\bar{h}\sum_{r=1}^{m}\frac{\bar{h}^{r-1}}{(r-1)!}+\bar{h}^2\sum_{r=2}^{m}\frac{\bar{h}^{r-2}}{(r-2)!}}{(m+1)(m+2)-2(m+1)\bar{h}+\bar{h}^2}$$

Proof

Write ψ_i for $\psi_i(h,y_n^{(m)})$ and $\bar{h}$ for $h\lambda$ where λ represents any eigenvalue of the initial problem whose solution we seek. By employing the normal scalar test equation $y^{(1)}=\lambda y$ and appealing to the result (2.14) – (2.18) above, the numerator of the classes of integrators reduces to

$$\lambda^{2m}y_n^3\left[-(m+1)(m+2)\sum_{r=0}^{m}\frac{\bar{h}^r}{r!}+2(m+1)\bar{h}\sum_{r=1}^{m}\frac{\bar{h}^{r-1}}{(r-1)!}-\bar{h}^2\sum_{r=2}^{m}\frac{\bar{h}^{r-2}}{(r-2)!}\right]\left[(m+1)!(m+2)!\right]^{-1}$$

while the denominator of the class of integrators reduces to :

$$\lambda^{2m}y_n^2\left[-(m+1)(m+2)+2(m+1)\bar{h}-\bar{h}^2\right]\left[(m+1)!(m+2)!\right]^{-1}$$

consequently the result (2.14) reduces to

$$y_{n+1}=\frac{\left[(m+1)(m+2)\sum_{r=0}^{m}\frac{\bar{h}^r}{r!}-2(m+1)\bar{h}\sum_{r=1}^{m}\frac{\bar{h}^{r-1}}{(r-1)!}+\bar{h}^2\sum_{r=2}^{m}\frac{\bar{h}^{r-2}}{(r-2)!}+\right]y_n}{(m+1)(m+2)-2(m+1)\bar{h}+\bar{h}^2}$$

For one step methods the stability function $s(\bar{h})$ is

defined by $s(\bar{h})=\dfrac{y_{n+1}(\bar{h})}{y_n(\bar{h})}$

Conclusively the required stability function is given by

$$s(\bar{h})=\frac{(m+1)(m+2)\sum_{r=0}^{m}\frac{\bar{h}^r}{r!}-2(m+1)\bar{h}\sum_{r=1}^{m}\frac{\bar{h}^{r-1}}{(r-1)!}+\bar{h}^2\sum_{r=2}^{m}\frac{\bar{h}^{r-2}}{(r-2)!}}{(m+1)(m+2)-2(m+1)\bar{h}+\bar{h}^2}$$

which is what we are required to establish.

Remarks (Region of absolute stability)

If the absolute value of the stability function of any one-step numerical integrator lies in the unit ball $/s(\bar{h})/<1,$ the region consisting of the values of $\bar{h}$ for which the state of $s(\bar{h})$ is attained is called the Region of Absolute Stability (RAS) of the integrator. In this class of integrators, $/s(h)/<1$, for the values of $m=0,1,2$ in the entire left half of the complex plane. Indeed for $m=0,1$ our integrator are L-stable while for $m=2,$ we have the integrator A-stable. The RAS shrinks as it grows larger. Writing $\bar{h}=u+iv$, where $i=\sqrt{-1},$ the left half of the complex plane is equal to the left half of $u-v$ plane.

Performance

We give in this section brief analysis and relevant results to indicate some of the immediate type of problems it can handle and those it cannot.

In order to avoid the use of extensive tables, we adopted the presentation of minima and maxima errors incurred in a given interval of operation. If there is any peculiarity, we state such lucidly. This approach saves time and space. In this regard, in a given interval $[a,b]$ on the real line R with $a<b,$ our representations are given as shown hereunder.

e = the error at a specified point in [a,b]
min (e) = the minimum error in [a,b]
max (e) = the maximum error in [a,b]

Theorem [Misleading constant value]

The new set of quadratic denominator-based integrators, in the case m = 0 produces misleading constant value whenever it is employed to solve any IVP where solution function passes through the origin while the gradient of the same solution function is not parallel to the axis of the independent variables at any point in [a,b].

Proof

At each point from our construction constraints,

$y(x_n) = y_n$ and $y^{(1)}(x_n) = y_n^{(1)}$

The set of Quadratic Denominator-based integrators is given by result (2.14) while the component interpretations are stated in results (2.15) – (2.18). Putting m = 0 in (2.14) – (2.18), we obtained

$$y_{n+1} = \frac{2y_n^3}{2y_n^2 - 2hy_ny_n^{(1)} + h^2\left[2(y_n^{(1)})^2 - y_n^{(2)}y_n\right]} \qquad (5.1)$$

If the solution of any given IVP

$$y^{(1)} = f(x, y), y(x_0) = y_0, x_0 E[a, b]$$

passes through the origin, then the given IVP has its initial values $y_0 = y(x_0)$ reducing to $y_0 = y(0) = 0;$ meaning $a = 0$.

Consequently, when we set $n = 0$ in result (5.1) above, we obtain the following results;

For numerator = $y_0^3 = 0$

Denominator = $2(hy_0^{(1)})^2$

Observe that $y^{(1)} = f(x, y)$ is the gradient of the solution function in $[a, b]$. That it is not parallel at to the axis of the independent variable in this case, the x-axis at the point x_n. Consequently $y_1 = 0$ if $y^{(1)} \neq o$ at $x = 0$. By induction step m, n, directly using the hypothesis of the theorem, we obtain $y_n = 0$ for every n provided the condition $f(x_n, y(x_n)) \neq 0$ for every n. Hence the integrator with $m = 0$ in the given set of the new integrator produces deceptively constant value at every point in the interval of integration $[a, b]$.

Remark

Theorem 1 above handles the situation wherein $y^{(1)}(x_n) \neq 0.$ The next theorem is a stronger form of theorem 1 in that it establishes the instability of the same integrator with $m = 0$ irrespective of whether $y^{(1)}(x_n) = 0$ or not.

Theorem 2

The quadratic Denominator-based set of integrators, in this case $m = 0$ is not suitable for implementing or obtaining the solution functions passing through the origin.

Proof

By theorem 1, we established the result in the case $y^{(1)} \neq 0$. Here we are left to consider the case $y^{(0)} = 0$. This is simply a case of zeros dividing zeros. Results from the fundamentals of real analysis has more three form to another to enable me arrive at whatever results could turn out to be. Hardly can one get a user who would simply prefer integrators that give quick result with less load of work.

RESULTS AND IMPLEMENTATION

Problem I

$$y^{(1)} = \begin{pmatrix} -2000 & 1000 \\ 1 & -1 \end{pmatrix} y + \begin{pmatrix} 1 \\ 0 \end{pmatrix}, y(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix} o \le x \le 5$$

$$TSOL = \begin{pmatrix} -4.998(-4) & -5.0025(-4) \\ 2.499(-7) & -1.000(-3) \end{pmatrix} \begin{pmatrix} e^{\lambda_1 t} \\ e^{\lambda_2 t} \end{pmatrix} + \begin{pmatrix} 1(-3) \\ 1(-3) \end{pmatrix},$$

where $a(b) = a \times 10^{-b}$

$$\lambda_1 = -2000.500125, \quad \lambda_2 = -0.499875$$

The stiff factor = $4(-4)$ and uniform $h = 0.005$.

In this problem we say that the solution passes through the origin (0,0). Indeed $y(0) = \begin{pmatrix} y_1(0) \\ y_2(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ and it is for the quadratic based denominator with *m = 1.* Table 1 shows the performance of the integrators against the theoretical solution (TSOL).

Theorem

The case *m= 0* cannot handle any IVP where solution function passes through the origin.

Proof

When *m = 0,* the integrator becomes

$$y_{n+1} = \frac{2y_n^3}{2y_n^2 - 2hy_ny_n^{(1)} + h^2\left[2(y_n^{(1)})^2 - y_n^{(2)}y_n\right]}$$

if the solution function passes through the origin then $y(0) = 0$ *iff* $y_0 = 0$.

Consequently, setting *n = 0* in this case yields

Table 1. The performance of the integrators against the theoretical solution (TSOL).

Errors in $o \leq x \leq 1$	Component 1	Component 2
min (e)	4.0(-5)	1.0(-4)
Max(e)	-4.1(-3)	-4.0(-4)

Table 2. Problem 2

Errors in [0,1] $0 \leq x \leq 1$	New Integrator $m = 2(p = 4)$	Fatunla $p = 3$	Niekerk I	Niekerk II	Luke et al
min(e) = 1.897(-6)	0.0	3E-6	1E-4	2E-6	1E-5
max(e) = -6.256(-2)	4E-4	4E-3	5E-1	2E-2	1E-1

Table 3. Problem 3

Error in $0 \leq x \leq 1$	New Integrator $m = 2$	Niekerek I
min(e)	0.0	0.0
max(e)	0.0	1.2E-4

$$y_1 = \frac{2y_0^3}{2y_0^2 - 2hy_0 y_0^{(1)} + h^2\left[2(y_0^{(1)})^2 - y_0^{(2)}\right] y_n}$$

$$y_1 = \frac{2y_0^3}{2y_0^2 - 2hy_0 y_0^{(1)} + h^2\left[2(y_0^{(1)})^2 - y_0^{(2)}\right] y_n}$$

$y_0 = 0$ does not necessarily implies $y_0^{(r)} = 0(\cancel{r}) \neq 0$.

Problem 2

$$y^{(1)} = 1 + y^2, \quad y(0) = 1.0, \quad 0 \leq x \leq 1.$$

$$\text{Tsol } y_0 = \tan(x + \frac{\Pi}{4}), \quad h = 0.05$$

The given problem has a singularity at $x = \frac{\Pi}{4}$, it shows that the new integration has improved performance of this class of integration against the other rational integrators in Table 2.

Problem 3

$$y^{(1)} = 1 + y^{(2)}, y(0) = 0, \qquad y = \tan x$$

In this case, $m = 0$ cannot handle this kind of problem (Table 3)

Table 4. Problem 4

Error in $0 \leq x \leq 3$	New Integrator $(m = 2, h = 0.0030)$	Rk4 $h = 0.030$
min(e) = 1.897(-6)	2E-6	6.7E-11
max(e) = 6.356(-2)	6E-2	1.9E-3

Table 5. Problem 5

H	N Steps	Integrator errors $(m = 2)$	Rk4
0.03	100	0.0	0.151007 -6.7×10^{11}
0.025	120	0.0	0.151007 0.150943
0.020	150	0.0	0.151007 -0.15007
0.015	200	0.0	0.15007 0.151004

Problem 4

$$y^{(1)} = -100(y - \sin x), y(0) = 0.0, \ 0 \leq x \leq 3.$$

Tsol is : Table 4.

In this case, the new integrator and with m = 2, copes favourably better with stiff and singular problems.

Problem 5

$$y^{(1)} = 100(y - \sin x)$$
$$y(0) = 0.0, \qquad 0 \leq x \leq 3.6$$

$$y(x) = \frac{\sin x - 0.01\cos x + 0.01\exp(-100x)}{1.0001}$$

Table 5

In this case when compared with Runge-Kutta of order 4, the new integrator has a higher degree of accuracy as attested by the number of steps under consideration.

Conclusion

The new integrator is L-stable and coped well with the classes of IVPs problem identified in this paper. The new integrator has a high degree of accuracy as they are tested compared favourably well with other conventional methods. It does not suffer from the problem associated with the predecessor integrators.

The integrator has the required A-stability and L-stability properties and the RAS of integrators covers the whole of the left-half of the complex plane.

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