

A ONE-STEP, FIFTH ORDER INTEGRATOR USING PADE RATIONAL FUNCTION FOR INITIAL VALUE PROBLEMS WITH SINGULAR SOLUTIONS AND STIFF DIFFERENTIAL EQUATIONS

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Abstract

The paper describes a one-step, fifth-order integrator well suited for the treatment of initial value problems with singular solution and stiff differential equations based on Pade rational function of order (M,N). Dalquist's model test equation was used to analyze its basic properties. The results show that the integrator is consistent and convergent. Numerical results and comparative analysis with some methods show that the integrator is very efficient and more accurate.

Introduction

The initial value problem given by

$$y' = f(x, y), y(x_0) = y_0, a \leq x \leq b \tag{1.1}$$

has solution function $y \in C[a, b]$, which may contain some discontinuities at some points in differential equations often known as points of discontinuities. There are many existing methods for the solution of initial value problems in differential equations based on rational approximations, which are quite effective for the solution of initial value problems with singular solution. However, the derivation of such methods is very tedious and complicated, Fatunla (1986). Also the performance of these methods near the singular point is not quite satisfactory. In view of these, we consider Pade rational approximation function of order (M, N) for the development of the integrator.

A Pade approximation of order M, N to an analytic function $f(x)$ at a regular point x_0 is the rational function $\frac{p(x)}{q(x)}$, where $p(x)$ is a polynomial of degree M , and $q(x)$ is a polynomial of degree N .

The Pade approximant is unique for given M and N , that is the coefficients a_i and b_j can be uniquely determined. Hence, we consider Pade rational approximant of the form:

$$\frac{\sum_{i=0}^M a_i x^i}{\sum_{j=0}^N b_j x^j}, M \geq 0, N \geq 0, 0 \leq i \leq M \text{ and } 0 \leq j \leq N \tag{1.2}$$

where a_i, b_j are real coefficients.

We define a finite difference numerical integrator of maximal order M for approximating initial value problem $y' = f(x, y), y(x_0) = y_0$ by

$$y_{i+1} = y_i + \frac{\Delta x}{1} \sum_{j=0}^M a_j f(x_i, y_i) \tag{1.3}$$

with $M \geq 0, N \geq 0, 0 \leq i \leq M$ and $0 \leq j \leq N$. The parameters a_i and b_j are constant coefficients to be determined (Wikipedia, 2009).

Derivation of One-Step, Fifth Order Integrator

The integrator we seek to develop is a one-step but of fifth-order method. This implies that the integrator is expected to use the value of y_i to compute y_{i+1} as an approximation to $y(x_{i+1})$, where $y(x)$ is the solution of the initial value problems $y' = f(x, y), y(x_0) = y_0$. Hence, if we take $M = 2, N = 3$ in equation (1.3), we have

$$y = \sum_{n=0}^{\infty} \frac{a_n}{n!} x^n \tag{2.1}$$

If we adopt Taylor series of y and ignore terms of order higher than 5 in equation (2.1), we obtain:

$$a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 = 0 \tag{2.2}$$

$$a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 = 0 \tag{2.3}$$

$$a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 = 0 \tag{2.4}$$

$$a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 = 0 \tag{2.5}$$

$$a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 = 0 \tag{2.6}$$

$$a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 = 0 \tag{2.7}$$

Taking (2.2) and equating the coefficients as far as x^5 , we have

$$a_0 = y \tag{2.2}$$

$$a_1 = y' \tag{2.3}$$

$$a_2 = y'' \tag{2.4}$$

$$a_3 = y''' \tag{2.5}$$

$$a_4 = y^{(4)} \tag{2.6}$$

$$a_5 = y^{(5)} \tag{2.7}$$

Solving for a_1, a_2 and a_3 in 2.5, 2.6 and 2.7, we have:

$$a_1 = \dots \tag{2.8}$$

where $\sum_{n=1}^3 \dots$ (2.9)

where $\sum_{n=1}^3 \dots$ (2.10)

where $\sum_{n=1}^3 \dots$ (2.11)

where $\sum_{n=1}^3 \dots$ (2.12)

where $\sum_{n=1}^3 \dots$ (2.13)

where $\sum_{n=1}^3 \dots$ (2.14)

where $\sum_{n=1}^3 \dots$ (2.15)

where $\sum_{n=1}^3 \dots$ (2.16)

where $\sum_{n=1}^3 \dots$ (2.17)

where $\sum_{n=1}^3 \dots$ (2.18)

Substituting a_1 in (2.3) and simplify, we have

$$a_1 = y' \tag{2.19}$$

$$a_1 = \frac{1}{20} \quad (2.15)$$

Substituting a_1 and a_2 in (2.4) and simplify, gives

$$a_2 = \frac{1}{20} y'' - \frac{1}{2} y''' - \frac{4}{20} y^{(4)} - \frac{10}{20} y^{(5)} \quad (2.16)$$

Substituting the values of a_0, a_1, a_2, a_3 and a_4 in (2.1), yields

$$y_1 = \frac{60}{60} y + \frac{12}{12} y' + \frac{3}{3} y'' + \frac{4}{4} y''' + \frac{10}{10} y^{(4)}, \quad (2.17)$$

Where

$$\sum_{i=1}^3 \frac{1}{i}$$

and the a_0, a_1, a_2, a_3 are as given in equations (2.11), (2.12), (2.16) and (2.17) respectively. Equation (2.17) is the required integrator.

Convergence of the Method

We establish the convergence of the integrator by showing that the integrator is consistent and stable.

Theorem 1: The one-step, fifth-order integrator (2.17) above is convergent, if and only if it is consistent.

Proof

A one-step numerical integrator of the form:

$y_1 - y_0 = \Delta t \Phi(\Delta t, y_0, y_0')$, is convergent if and only if it is consistent

If we subtract y_0 from both sides of (2.17), we have

$$y_1 - y_0 = \frac{60}{60} y_0 + \frac{12}{12} y_0' + \frac{3}{3} y_0'' + \frac{4}{4} y_0''' + \frac{10}{10} y_0^{(4)} - y_0 \quad (3.1)$$

Hence

$$\frac{60}{60} y_0 + \frac{12}{12} y_0' + \frac{3}{3} y_0'' + \frac{4}{4} y_0''' + \frac{10}{10} y_0^{(4)} - y_0 \quad (3.2)$$

Then

$$\lim_{\Delta t \rightarrow 0} \frac{60}{60} y_0' = y_0' \quad (3.3)$$

This implies that

$$\lim_{\Delta t \rightarrow 0} \frac{60}{60} y_0' \cong y_0'$$

This implies that the integrator is consistent with the initial value problem $y' = f(t, y), y_0 = y_0$. Hence the integrator is convergent.

Theorem 2: The integrator (2.17) is L-Stable

Proof

If we apply to the integrator (20), the well-known Dahlquist stability test equation

$$y' = \lambda y, y_0 = y_0 \text{ and } \lambda = 0. \quad (3.4)$$

We obtain finite difference equations

$$\begin{array}{l}
 1 \quad - y^3 \\
 2 \quad 18 y^3 \\
 3 \quad 20 y^3 \\
 \quad \quad 37 y^3 \\
 1 \quad - 6 y^3 \\
 2 \quad - 12 y^3 \\
 3 \quad - 6 y^3 \\
 \quad \quad - 19 y^3 \\
 t_1 \quad - 2 y^3 \\
 2 \quad 9 y^3 \\
 3 \quad - 10 y^3 \\
 \quad \quad - 3 y^3 \\
 r_1 \quad - 3 y^3 \\
 2 \quad 6 y^3 \\
 3 \quad - 10 y^3 \\
 \quad \quad - 7 y^3
 \end{array}$$

Then

$$y_1 = \frac{1140 \quad 1104 \quad 423}{1140 \quad 36 \quad 111} y \tag{3.5}$$

If we set α in (3.5), then we have

$$y_1 = \frac{1140 \quad 1104 \quad 423}{1140 \quad 36 \quad 111} y \tag{3.6}$$

Also, we put:

$$\alpha = \dots$$

Then

$$\alpha = \frac{1140 \quad 1104 \quad 423}{1140 \quad 36 \quad 111} \tag{3.7}$$

Hence

$$\lim_{\alpha \rightarrow \infty} \alpha = 0$$

Therefore the integrator is L-Stable.

Implementation of the Integrator

Problem 1: $y' = 1 - y^2, y(0) = 1$

The theoretical solution is $y = \tan(\pi/4 - x)$ with singular point at $\pi/4$. Taking $\alpha = 0.05$, we have the performance of the integrator in table 1 compared with the exact solution and the results of other methods.

Table 1: Shows the performance of the integrator against the exact solution, compared with Fatunla(1986), Okoson and Ademiluyi (2007).

X	Exact solution	New scheme	Fatunla(1986)	Okosun& Ademiluyi(2007)	Error of new method
0	1.0000000000000000	1.0000000000000000	1.0000000000000000	1.0000000000000000	0
0.05	1.105355590485906	1.105355590640578	1.1111111111111111	1.104972375690608	1e-10
0.10	1.223048880449865	1.223048880780532	1.235330450895615	1.222248400788326	1e-10

0.15	1.356087851147709	1.356087851684872	1.376016469816330	1.354812994785801	3e-10
0.20	1.508497647121400	1.508497647908448	1.537684974287252	1.506660406267608	6e-10
0.25	1.685796417168340	1.685796418267518	1.726573228313592	1.683264643925649	1e-09
0.30	1.895765122854009	1.895765124356339	1.951564752192567	1.892339969539771	2e-09
0.35	2.149747640196674	2.149747642239140	2.225777678561865	2.145123885181703	6e-09
0.40	2.464962756722603	2.464962759519616	2.569449049356346	2.458655513403594	1e-08
0.45	2.868884028016388	2.868884031921410	3.015544156807407	2.860084130839139	5e-08
0.50	3.408223442335828	3.408223447973148	3.621657355264633	3.395486432594335	2e-08
0.55	4.169364045966011	4.169364054546901	4.498331302620708	4.149860092867905	2e-07
0.60	5.331855223458727	5.331855237671617	5.888113262972766	5.299248116897016	1e-07
0.65	7.340436575043412	7.340436602237845	8.446551225886461	7.277274507461184	3e-07
0.70	11.681373800310224	11.681373869653310	14.773080772272847	11.518086957916351	9e-06
0.75	28.238252850141599	28.238253257270571	57.268565089739333	27.276367141591592	5e-06
0.80	-68.479668345576044	-68.479665944871840	-30.718513177654096	-75.110865861177430	6e-05
0.85	-15.457896135509500	15.457896001660210	-12.105563525031847	-15.783873157672124	2e-05
0.90	-8.687629546481706	8.687629504203230	-7.521746940402024	8.793873715546377	3e-08
0.95	-6.020299716350468	-6.020299696076126	-5.439761313908228	-6.073487193506408	6e-08
1.00	-4.588037824983901	-4.588037813245333	-4.245900513013902	-4.620467390357177	8e-09

Analysis of Results

The problem was solved numerically with the integrator (2.17) and the results are shown in table 1. It can be seen that the discretisation errors e_n obtained from the solution are sufficiently small, because of the stability property of the formula and its performance near the singular point is near accurate and it is the best when compared to the other methods developed earlier on.

Problem 2:

Taking uniform step size $h = \frac{1}{40}$, the performances of the new integrator are shown in table 2 compared with the exact solution and Fatunla (1986) and Okosun and Ademiluyi (2007).

Table 2: Shows the performance of the new integrator against the exact solution, compared with Fatunla (1986) and Okosun and Ademiluyi (2007).

X	Exact solution	New scheme	Fatunla (1986)	Okosun & Ademiluyi (2007)	Error of new method
0	1.000000000000000	1.000000000000000	1.00000	1.000000000000000	0
/40	0.996917333733128	0.996917333244523	1.00000	0.996925231982148	5e-09
2/40	0.987688340595138	0.987688339128452	1.00000	0.987743545594948	1e-09
3 /40	0.972369920397677	0.972369917704661	1.00000	0.972524195024528	3e-09
4 /40	0.951056516295154	0.951056512206082	1.00000	0.951367215342461	6e-09
5 /40	0.923879532511287	0.923879526894595	1.00000	0.924408912954045	1e-09
6 /40	0.891006524188368	0.891006516934439	1.00000	0.891822474925154	2e-09
7 /40	0.852640164354092	0.852640155366828	1.00000	0.853817715486277	6e-09
8 /40	0.809016994374947	0.809016983566406	1.00000	0.810640595179367	1e-08
9 /40	0.760405965600031	0.760405952886281	1.00000	0.762572770888364	5e-08
10 /40	0.707106781186548	0.707106766483764	1.00000	0.709931421558867	2e-08
11 /40	0.649448048330184	0.649448031550292	1.00000	0.653069712728592	2e-08
12 /40	0.587785252292473	0.587785233337577	1.00000	0.592378533209569	1e-08
13 /40	0.522498564715949	0.522498543470473	1.00000	0.528290699751432	3e-08
14 /40	0.453990499739547	0.453990476058231	1.00000	0.461290039331072	9e-08
15 /40	0.382683432365090	0.382683406053280	1.00000	0.391930549471038	5e-08
16 /40	0.309016994374947	0.309016965153493	1.00000	0.320877770812029	6e-08
17 /40	0.233445363855905	0.233445331292006	1.00000	0.249003354369111	2e-08
18 /40	0.156434465040231	0.156434428390341	1.00000	0.177620342030789	3e-08
19 /40	0.078459095727845	0.078459053491079	1.00000	0.109131277544694	6e-08

18 /40	0.000000000000000	-0.000000052031308	1.00000	0.048932492909149	8e-07
19 /40	-0.078459095727845	-0.078459205626557	1.00000	0.009453197092404	1e-07
20 /40	-0.156434465040231	0.156434559452170	1.00000	0.000120680617528	5e-07
21 /40	-0.233445363855905	-0.233445450418596	1.00000	0.00000000284489	2e-07
22 /40	-0.309016994374947	-0.309017074980805	1.00000	0.000000000000000	2e-07
23 /40	-0.382683432365090	-0.382683507720342	1.00000	0.000000000000000	1e-07
24 /40	-0.453990499739547	-0.453990570122491	1.00000	0.000000000000000	3e-07
25 /40	-0.522498564715949	-0.522498630212152	1.00000	0.000000000000000	9e-07
26 /40	-0.587785252292473	-0.587785312891945	1.00000	0.000000000000000	5e-07
27 /40	-0.649448048330184	0.649448103975197	1.00000	0.000000000000000	6e-07
28 /40	-0.707106781186547	-0.707106831798281	1.00000	0.000000000000000	2e-07
29 /40	-0.760405965600031	-0.760406011094933	1.00000	0.000000000000000	3e-08
30 /40	-0.809016994374947	-0.809017034675713	1.00000	0.000000000000000	2e-08
31 /40	-0.852640164354092	-0.852640199397710	1.00000	0.000000000000000	2e-08
32 /40	-0.891006524188368	-0.891006553932683	1.00000	0.000000000000000	6e-08
33 /40	-0.923879532511287	-0.923879556941144	1.00000	0.000000000000000	2e-08
34 /40	-0.951056516295154	0.951056535429291	1.00000	0.000000000000000	3e-08
35 /40	-0.972369920397677	-0.972369934298337	1.00000	0.000000000000000	5e-08
36 /40	-0.987688340595138	0.987688349385201	1.00000	0.000000000000000	1e-08
37 /40	-0.996917333733128	-0.996917337637150	1.00000	0.000000000000000	5e-07
38 /40	-1.000000000000000	-0.999999999507400	1.00000	0.000000000000000	e-09
39 /40					

Analysis

Problem 2 was also solved using the integrator (2.17) the results are shown in tables 2. It could be seen in table 2 that the results of the new methods are almost as the same as the exact solution. Fatunla(1986) and Okosun and Ademiluyi(2007) could not cope with this class of problems. The new integrator performs better because it is capable of solving oscillatory problems and initial value problems with singular solutions as well as stiff differential equations.

Problem 3: Solve the stiff equation $y' - 20y = 1$, $y(0) = 1$

The theoretical solution is $y = \frac{1}{20} + e^{-20x}$. Taking $h = 0.1$, we have the performance of the integrator in table 3 below.

Table 3: Shows the performance of our integrator against the exact solution, compared with Euler methods

X	Exact solution	New scheme	Explicit Euler method h=0.1	Implicit Euler method h=0.1	Error
0	1.000000000000000	1.000000000000000	1.000000000000000	1.000000000000000	0
0.1	0.135335283236613	0.135135135135135	-1.000000000000000	0.333333333333333	2e-04
0.2	0.018315638888734	0.018261504747991	1.000000000000000	0.111111111111111	5e-04
0.3	0.002478752176666	0.002467770911891	-1.000000000000000	0.037037037037037	1e-05
0.4	0.000335462627903	0.000333482555661	1.000000000000000	0.012345679012346	1e-06
0.5	0.000045399929762	0.000045065210224	-1.000000000000000	0.004115226337449	3e-07
0.6	0.000006144212353	0.000006089893274	1.000000000000000	0.001371742112483	5e-08
0.7	0.000000831528719	0.000000822958550	-1.000000000000000	0.000457247370828	8e-09
0.8	0.000000112535175	0.00000011210615	1.000000000000000	0.000152415790276	1e-09
0.9	0.000000015229980	0.000000015028461	-1.000000000000000	0.000050805263425	2e-10
1.0	0.000000002061154	0.000000002030873	1.000000000000000	0.000016935087808	3e-11

Analysis of Results

The performance of the new integrator on stiff differential equation is promising. As we can see in table 3 the performance of the new integrator is better than that of the implicit Euler method which is known to cope with stiff differential equations.

Conclusion

The theoretical analysis showed that the integrator is a good numerical method for the treatment of singular initial value problems and also effective in treating stiff differential equations.

The method will therefore be useful in the solution of problems arising from electrical networks, chemical kinetics, control theory, economy affected by inflations and population growth problems.

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