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A sixth-order exponentially fitted scheme for the numerical solution of systems of ordinary differential equations

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Abstract

A class of sixth-order three-step second derivative scheme is developed for stiff systems of ordinary differential equations. The numerical stability analysis of the scheme revealed that, it is A-stable. The result of some standard numerical examples are presented which allow an appraisal of the proposed scheme with existing methods.

Mathematics Subject Classification : 65L05, 65L06, 65L20 Keywords: Three-step second derivative, exponentially fitted, stiff systems, *A*-stable.

1 Introduction

We shall be concerned with the numerical solution of stiff systems of ordinary differential equation of the form

$$y' = f(x, y);$$
 $y(x_0) = y_0$ (1.1)

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where $x \in [a, b], y, f \in \mathbb{R}^n$. The idea of using exponentially fitted methods which originally proposed by Liniger and Willoughby [9], derived one-step integration formula containing free parameters for stiff systems denoted by F^r , r = 1, 2, 3, where the index 'r' represent the order of the method. These formulas were shown to be A-stable for certain choices of the fitting parameters. In the same way, Jackson and Kunue [8] designed a fourth-order exponentially fitted formula denoted by F^4 based on a linear two-step method which is $A(\alpha)$ stable, for ' α ' very near $\pi/2$. Cash[4] used the F^4 as a predictor to develop a fifth-order composite second derivative linear multistep method, he discovered the absence of A-stability. Voss[10] also utilized F^4 to derived a fifth-order second derivative method for stiff systems which he found to be A-stable, Abhulimen and Otunta [1, 2, 3] in the spirit of Cash[4] developed two-step third derivative exponentially fitted methods of orders 7,8 and 9, denoted by AB7, AB8, NM9 respectively. These methods were found to be compatible with A-stability for all choices of fitting parameters.

However, the aim of this present paper is to develop three-step second derivative exponentially fitted scheme of order six which is A-stable for all choices of fitting parameters.

Remark 1.1. It is important to note that for systems for which exponential fitting is appropriate, it is usually found that exponentially fitted integration formulas are substantially more efficient than conventional ones.

Remark 1.2. The exponential fitting methods also offer favourable properties in the integration of differential equations whose Jacobian has large imaginary eigenvalues Hochbruck, et al. [7].

2 Derivatives of the scheme

We consider the multiderivative multistep for the initial value problems 1.1;

$$\sum_{t=0}^{k} \left[a_t y_{n+t} - \sum_{q=1}^{p} h^q \gamma_{qt} y_{n+t}^q \right] = 0$$
 (2.1)

where k, p, and q are positive integers, h > 0 is a step-size independent of n, y_{n+t} are approximate to $y(x_{n+t})$, $x_{n+t} = (n+t)h$. The coefficients a_t , γ_{qt} are real constants subject to the conditions, $a_k = 1$, $|a_0| + |\gamma_{q0}| \neq 0$. **Remark 2.1.** If k = 1 Equation 2.1 is called one-step method. So, when k = 3, and h = 2, we referred to it as three-step second derivative method, which is our major focus in this paper.

For purpose of efficient implementation of the new proposed scheme, we adopt the mechanism in Cash [4] and Abhulimen and Okunuga [3] by splitting 2.1 into predictor and corrector schemes as follows:

$$\sum_{t=0}^{k} a_t y_{n+t} - \left[h \sum_{t=0}^{k} b_t y'_{n+t} + h^2 \sum_{t=0}^{k} d_t y''_{n+t} \right] = 0$$
(2.2)

and

$$\sum_{t=0}^{k} a_t y_{n+t} - \left[h \sum_{t=0}^{k+1} b_t y'_{n+t} + h^2 \sum_{t=0}^{k} d_t y''_{n+t} \right] = 0$$
(2.3)

where $b_t = \gamma_{1,t}$, $d_t = \gamma_{2,t}$, $y'_{n+t} = y^{(1)}_{(x_n+t)}$; $y''_{n+t} = y^{(2)}_{(x_n+t)}$. Then Equations 2.2 and 2.3 serves as predictor and corrector respectively.

Remark 2.2. When deriving exponentially fitted methods, the approach is to allow both 2.2 and 2.3 to possess free parameters which allow it to be fitted automatically to exponential functions.

To derive our predictor method of order six, we employed the Taylor series expansion to (2.2), to obtain a set of six equations. We let $b_3 = r$ (as free parameter) and $a_k = a_3 = 1$ (since k = 3), we have

$$a_{0} + 1 = 0$$

$$3(1 - \frac{r}{3}) - (b_{1} + b_{2}) = b_{0}$$

$$\frac{1}{2}(9 - 6r) - (b_{1} + 2b_{2} + d_{3}) = d_{0}$$

$$9(1 - r) - (4b_{2} + 6d_{3}) = b_{1}$$

$$\frac{1}{32}(81 - 108r) - \frac{1}{32}[4b_{1} + 108d_{3}] = b_{2}$$

$$\frac{1}{20}(9 - 15r) - \frac{1}{180}(b_{1} + 16b_{2}) = d_{3}$$

$$(2.4)$$

We then solve for the values of the unknown parameters, and substituting these values into 2.2, we obtain the three-step second derivative predictor method of order six.

$$y_{n+3} = y_n + h \left[\left(\frac{39}{40} - r\right) y'_n + \left(\frac{39}{13}r\right) y'_{n+1} + \left(\frac{81}{40} - \frac{27}{13}r\right) y'_{n+2} + ry'_{n+3} \right] (2.5) + h^2 \left[\left(\frac{3}{10} - \frac{6}{13}r\right) y''_n + \left(\frac{3}{20} - \frac{6}{13}r\right) y''_{n+3} \right]$$

Next, we introduce the scalar test function for the purpose of exponential fitting and stability analysis of our methods as follows: Let

$$y'_{(x)} = \lambda y(x); \qquad y(0) = 1$$
 (2.6)

where $Re(\lambda) < 0$.

When we apply (2.5) to (2.6), we obtain the exponential fitted predictor scheme of order six.

$$\frac{\bar{y}_{n+3}}{y_n} = \frac{1 + (\frac{39}{40} - r)u + (\frac{27}{13}r)ue^u + (\frac{81}{40} - \frac{27}{13}r)ue^{2u} + (\frac{3}{10} - \frac{6}{13}r)u^2}{1 - ru - (\frac{3}{10} - \frac{6}{13}r)u^2} = \bar{R}(u)$$
(2.7)

where $u = \lambda h$.

Similarly, to derive the three-step corrector method of order six, we maintain the same condition as in the case of predictor and let $b_4 = s$ (free parameter), we then have seven sets of equations as follows:

$$a_{0} + 1 = 0$$

$$3(1 - \frac{1}{3}s) - (b_{1} + b_{2}) = b_{0}$$

$$\frac{1}{2}(9 - 8s) - (b_{1} + 2b_{2} + d_{3}) = d_{0}$$

$$\frac{1}{3}(27 - 48s) - (4b_{2} + 9b_{3} + 6d_{3}) = b_{1}$$

$$\frac{1}{32}(27 - 256s) - \frac{1}{8}(b_{1} + 27b_{3} + 27d_{3}) = b_{2}$$

$$\frac{1}{81}(121s - 256s) - \frac{1}{81}(b_{1} + 16b_{2} + 16d_{3}) = b_{3}$$

$$\frac{1}{270}(243 - 2048s) - \frac{1}{270}(2b_{1} + 64b_{2} + 486b_{3}) = d_{3}$$

$$(2.8)$$

As before, after determining the values of the unknown parameters, we substitute the values into (2.3) to obtain the corrector formula

$$y_{n+3} = y_n + h \left[\left(\frac{39}{80} - \frac{29}{9} s \right) y'_n + \left(\frac{81}{80} + 8s \right) y'_{n+1} + \left(\frac{81}{80} - 12s \right) y'_{n+2} + \left(\frac{39}{80} + \frac{56}{9} s \right) y'_{n+3} + s y'_{n+4} \right] + h^2 \left[\left(\frac{3}{40} - \frac{4}{3} s \right) y''_n + \left(-\frac{3}{40} - \frac{16}{3} \right) y''_{n+3} \right]$$

$$(2.9)$$

We apply (2.9) to (2.6) to obtain the exponentially fitted corrector method of order six.

$$\frac{y_{n+3}}{y_n} = \frac{1 + us(e^{4u}) + (\frac{81}{80} - 12s)ue^{2u} + (\frac{89}{80} + 80s)ue^u + (\frac{89}{80} - \frac{29}{9}s)u + (\frac{3}{40} - \frac{4}{3}s)u^2}{1 - (\frac{39}{80} + \frac{56}{9}s)u - (-\frac{3}{4} - \frac{16}{3}s)u^2} = R(u) \quad \text{say}$$

$$(2.10)$$

However, for purpose of computation and stability analysis, we unite the predictor (2.7) and the corrector (2.10) together to obtain;

$$\frac{y_{n+3}}{y_n} = \frac{1 + us[\bar{R}(u)]^{4/3} + (\frac{81}{80} - 12s)u[\bar{R}(u)]^{2/3} + (\frac{81}{80} + 80s)u[\bar{R}(u)]^{1/3}}{1 - (\frac{29}{80} + \frac{56}{9}s)u - (-\frac{3}{4} - \frac{16}{3}s)u^2} + \frac{(\frac{89}{80} - \frac{29}{9}s)u + (\frac{3}{40} - \frac{4}{3}s)u^2}{1 - (\frac{29}{80} + \frac{56}{9}s)u - (-\frac{3}{4} - \frac{16}{3}s)u^2}$$
(2.11)

where

$$e^{4u} = \frac{y_{n+4}}{y_n} = \left[\frac{\bar{y}_{n+3}}{y_n}\right]^{4/3} = [\bar{R}(u)]^{4/3}$$
$$e^{2u} = \frac{y_{n+2}}{y_n} = \left[\frac{\bar{y}_{n+3}}{y_n}\right]^{2/3} = [\bar{R}(u)]^{2/3}$$
$$e^u = \frac{y_{n+1}}{y_n} = \left[\frac{\bar{y}_{n+3}}{y_n}\right]^{1/3} = [\bar{R}(u)]^{1/3}$$

3 Stability Analysis

Definition 3.1. A numerical method is said to be A-stable if its reguin of absolute stability (RAS), contains the whole of the left-half of the complex plane. That is h > 0 for all values of $Re(\lambda h)$ is negative.

Now, to investigate the stability criteria of our method, the determination of the values of the free parameter r(u) and s(u) in the open left-half plane $(-\infty, 0]$ becomes very important. From equations (2.7) and (2.10), we obtain the free parameters r(u) and s(u) respectively as follows:

$$r(u) = \frac{1 + \frac{1}{40}u(39 + 81e^{2u}) + \frac{3}{10}u^2(1 + \frac{1}{2}e^{3u}) - e^{3u}}{\frac{29}{13}u(e^{2u} + e^u) + \frac{6}{13}u^2(1 + e^{3u}) + u(1 - e^{3u})}$$
(3.1)

and

$$s(u) = \frac{1 + \frac{81}{80}u(e^{2u} + e^u) + \frac{59}{80}u(1 + e^{3u}) + \frac{3}{40}u^2(1 - e^{3u}) - e^{3u}}{4u(3e^{2u} - 2e^u) + \frac{1}{9}u(29 - 56e^{3u}) + \frac{4}{3}u^2(1 + 4e^{3u}) - ue^{4u}}$$
(3.2)

By Cash[4] mechanism, we need to find the conditions which r(u) and s(u) needs to satisfy such that

$$\left|\frac{y_{n+2}}{y_n}\right| < 1, \quad \text{i.e.} \quad |R(u)| < 1$$
 (3.3)

for all u, with Re(u) < 0.

Necessary and sufficient conditions this inequality (3.3) to hold are given by the application of the maximum modulus theorem

- (i) $|R(u)| \le 1$ in Re(u) = 0.
- (ii) R(u) analytic in Re(u) < 0.

If condition (i) holds, it follows that R(u) is analytic at $u = -\infty$ and thus (i) and (ii) will guarantee A-stability by the maximum modulus theorem.

From (3.3) $-1 < \frac{y_{n+3}}{y_n} < 1$, but it is obviously true for $-1 < \frac{y_{n+3}}{y_n}$, we are now left with the case of

$$\frac{y_{n+3}}{y_n} < 1$$
 i.e. $R(u) < 1$ (3.4)

Now, from equation (3.4), we have

$$\frac{y_{n+3}}{y_n} - 1 < 0 \quad \text{i.e.} \quad R(u) - 1 < 0 \tag{3.5}$$

From equation (2.10), we have that

$$\frac{1 + us[\bar{R}(u)]^{34} + A_1 ue^{2u} + A_2 ue^u + A_3 u + A_4 u^2}{1 - B_1 u - B_2 u^2} - 1 < 0$$
(3.6)

where $A_1 = \frac{81}{80} - 12s$, $A_2 = (\frac{89}{80} + 80s)$, $A_3 = (\frac{89}{80} - \frac{29}{9}s)$, $A_4 = (\frac{3}{40} - \frac{4}{3}s)$, $B_1 = (\frac{39}{80} + \frac{56}{9}s)$, $B_2 = (-\frac{3}{40} - \frac{16}{3}s)$.

So, it becomes easy to verify that as $u \to -\infty$ for our problem (3.5), condition (i) gives

$$\frac{3}{40} - \frac{4}{3}s < 0$$

$$s < \frac{9}{180}$$
(3.7)

Similarly, we need to check the conditions satisfy by r

$$\frac{\bar{y}_{n+3}}{y_n} - 1 < 0$$

i.e.

i.e.

$$\bar{R}(u) - 1 < 0$$
 as $u \to -\infty$

From (2.7), we have

$$\frac{1+D_1u+D_2ue^u+D_3ue^{2u}+D_4u^2}{1-ru-Fu^2}-1<0$$
(3.8)

where $D_1 = (\frac{39}{40} - r), D_2 = \frac{27}{13}r, D_3 = (\frac{81}{40} - \frac{29}{13}r), D_4 = (\frac{3}{10} - \frac{6}{13}r), F = (\frac{3}{10} - \frac{6}{13}r).$ Again as $u \to -\infty$, we obtain the inequality

$$\frac{3}{10} - \frac{6}{13}r < 0$$

$$r < \frac{13}{20}$$
(3.9)
(3.9)

Thus (3.7) and (3.9) will help to determine the region of absolute stability of our proposed scheme. We further show that r(u) and s(u) have finite limit at origin and infinity.

From (3.1)

$$\lim_{u \to -\infty} r(u) = \frac{13}{20}$$
 and $\lim_{u \to 0} r(u) = 0$

In similar fashion, from (3.2), we obtain

$$\lim_{u \to -\infty} s(u) = \frac{9}{160} \quad \text{and} \quad \lim_{u \to 0} s(u) = -\frac{523}{1760}$$

Thus

i.e.

$$r \in [\frac{13}{20}, 0]$$
 and $s \in [\frac{9}{160}, -\frac{523}{1760}]$ (3.10)

These interval becomes the region of absolute stability.

We further use numerical procedure to examine the behaviour of our parameters by plotting the values of r(u) and s(u) for a large sample of u in the range $(-\infty, 0]$ as shown in Table (3.1) below.

Table 3.1: Parameter values of r and s as a function of u.

u	r	s
-10.0	0.587751	0.035846
-50.0	0.636185	0.031738
-100.0	0.643024	0.0539733
-1000.0	0.649296	0.056021
-2000.0	0.649648	0.056135
-3000.0	0.649650	0.056147
-4000.0	0.649660	0.056152
-5000.0	0.649672	0.056165
-6000.0	0.649683	0.056178
-7000.0	0.649689	0.056182
-8000.0	0.649660	0.056188
-9000.0	0.649661	0.056200
-10000.0	0.650000	0.056245

From Table (3.1), we observed that as the values of u decreases, the values of the parameters r(u) and s(u) are monotonically increasing. This suggests that all values of r(u) and s(u) within these ranges are convergent and bounded.

Theorem 3.2. A monotonic increasing sequence of real set of numbers which is bounded above converges.

Thus the set of values in Table (3.1) will satisfy the A-stability condition given by maximum modulus theorem.

Finally, it remains to investigate whether condition (ii) of the maximum is satisfied for all $u \in (-\infty, 0]$. Now the stability function of our new proposed scheme from equation (2.11) is given by

$$\begin{split} \tau^2 &= \frac{1+us[\bar{R}(u)]^{3/4}+(\frac{81}{80}-12s)u[\bar{R}(u)]^{2/3}+(\frac{81}{80}+80s)u[\bar{R}(u)]^3}{1-(\frac{39}{80}+\frac{56}{9}u)-(-\frac{3}{4}-\frac{16}{3}s)u^2} + \\ &+ \frac{(\frac{81}{80}-\frac{29}{9}s)u+(\frac{3}{40}-\frac{4}{3}s)u^2}{1-(\frac{39}{80}+\frac{56}{9}u)-(-\frac{3}{4}-\frac{16}{3}s)u^2} \end{split}$$

Evaluating for all values of $u \in (-\infty, 0]$ in the stability function, we established that $|\tau| < 1$ for all i.e. $\frac{y_{n+3}}{y_n} < 1$ for all Re(u) < 0. Hence our new proposed exponential fitted scheme of order six is A-stable for choices of the fitting parameters.

4 Numerical Examples and Results

In other to appraise the efficiency and accuracy of our new scheme, we present some numerical examples and results in this section. The implementation of our new scheme was carried out in double precision on FORTRAN on digital desktop computer.

Example 4.1. We consider Ehle's linear problem [5].

$$y' = -y + 95z;$$
 $y(0) = 1$
 $z' = -y - 97z;$ $z(0) = 1$
 $x \in [0, 1]$

The eigenvalues of the Jacobian at x = 0 are $\lambda_1 = -2$ and $\lambda_2 = -96$.

Example 4.2. Test problem from Enright and Pryce[6]

$$y'_{1} = -10^{4}y_{1} + 100y_{2} - 10y_{3} + y_{4}; \qquad y_{1}(0) = 1$$
$$y'_{2} = -100y_{2} + 10y_{3} - 10y_{4}; \qquad y_{2}(0) = 1$$
$$y'_{3} = -y_{3} + 10y_{4}; \qquad y_{3}(0) = 1$$
$$y_{4} = -0.1y_{3}; \qquad y_{4}(0) = 1$$

The eigenvalues of Jacobian are $\lambda_1 = -0.1$, $\lambda_2 = -1.0$, $\lambda_3 = -10000.0$, $\lambda_4 = -10000.0$.

Example 4.3. Second order differential equation taken from Abhulimen and Okunuga[3]

$$y'' + 1001y' + 100y = 0$$
$$y(0) = 1, y'(0) = 1$$

The eigenvalues of the Jacobian are $\lambda_1 = -1$ and $\lambda_2 = -1000$.

The results obtained for the integration of Example 4.1 using fixed stepsizes are given in Table 4.1. Here $F^{(4)}$, CH4, CH5, and $F^{(5)}$ denote the formulas due to Jackson and Kunue, Cash's method of order 4 and 5, and formula due to Voss David respectively. While AB7, AB8 and NM9(represent Abhulimen and Otunta two-step third derivative methods of order seven, eight and nine respectively. $F^{(6)}$ denote our proposed three-step second derivative scheme.

Table 4.1a: Efficiency and accuracy of new the integrator scheme on Problem 1 at x = 1.

step	method	y(1) (error)	$z(1) \times 10^2 (\text{error} \times 10^2)$
0.0625	CH4	$0.27355498(3.0 \times 10^{-7})$	$-0.2879471(3.0 \times 10^{-7})$
	CH5	$0.27355005(1.0 \times 10^{-8})$	$-0.28794742(1.0 \times 10^{-8})$
	AB7	$0.27354004(4.0 \times 10^{-5})$	$-0.28796321(6.0\times10^{-5})$
	F^4	$0.2735503(3.0 \times 10^{-7})$	$-0.2879477(3.1 \times 10^{-7})$
	NM9	$0.27354004(7.9 \times 10^{-5})$	$-0.28794740(8.3 \times 10^{-7})$
	F^5	$0.27355003(6.4 \times 10^{-9})$	$-0.28794741(6.7 \times 10^{-9})$
	$*F^6$	$0.29355004(3.2 \times 10^{-10})$	$-0.28794748(2.4 \times 10^{-10})$

		at $x = 1$.	
step size	method	y(1) (error)	$z(1) \times 10^2 (\text{error} \times 10^2)$
0.03125	CH4	$0.27355003(1.0 \times 10^{-8})$	$-0.28794742(1.0 \times 10^{-8})$
	NM9	$0.27354004(3.7 \times 10^{-5})$	$-0.28794744(4.0\times10^{-5})$
	F^4	$0.27355005(1.0 \times 10^{-8})$	$-0.28794742(1.0 \times 10^{-8})$
	F^5	$0.27355004(6.3 \times 10^{-10})$	$-0.28794740(1.4 \times 10^{-10})$
	$*F^6$	$0.27355005(1.2 \times 10^{-10})$	$-0.28794741(8.1 \times 10^{-10})$
	True solution	0.27355004	$-0.28794741 \times 10^{-2}$

Table 4.1b: Efficiency and accuracy of new integrator scheme on problem 1

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From the numerical results of Example 4.1 presented in Table (4.1a) and (4.1b), we observed at step size h = 0.0625, our proposed scheme have higher accuracy. And for h = 0,03125 our new scheme compete favourably with the existing methods.

 Table 4.2: Absolute error of Numerical solution of Example 4.2.

step	method	$y_1(1)$	$y_2(1)$	$y_3(1)$	$y_4(1)$
0.05	AB7	3.2×10^{-2}	3.2×10^{-2}	3.3×10^{-1}	3.7×10^{-5}
	NM9	$2.2 imes 10^{-3}$	$3.5 imes 10^{-2}$	3.2×10^{-5}	$3.2 imes 10^{-6}$
	$*F^6$	$3.5 imes 10^{-5}$	$3.8 imes 10^{-4}$	$3.5 imes 10^{-7}$	$3.7 imes 10^{-8}$
0.1	AB7	2.5×10^{-2}	2.1×10^{-1}	-2.4×10^{-3}	2.7×10^{-5}
	NM9	$2.7 imes 10^{-3}$	2.4×10^{-3}	-2.2×10^{-4}	2.5×10^{-6}
	$*F^6$	$2.9 imes 10^{-5}$	$2.7 imes 10^{-4}$	-2.6×10^{-6}	$2.6 imes 10^{-8}$

The true solution is given by

$$y_1(1) = -5911.9073$$

$$y_2(1) = -596.61978$$

$$y_3(1) = 5.3695798$$

$$y_4(1) = 0.05966201.$$

Remark 4.4. Example 4.2 was considered by Enright and Pryce[6] and the error tolerance was fixed at 10^{-5} . However, the results obtained by $*F^6$ shows that the error can be raised to 10^{-8} as against 10^{-5} given by Enright and Pryce [6]. We further observed form Table (4.2) that the results obtained by $*F^6$ at x = 1 for both h = 0.05 and 0.1, show that our method is more accurate.

step	method	y(x)	(error-)
0.05	AF5	0.36787930	1.8×10^{-7}
	AB7	0.36787840	1.7×10^{-6}
	$*F^6$	0.36787846	1.4×10^{-8}
0.125	AB5	0.36780800	1.4×10^{-6}
	$*F^6$	0.36789400	$1.4 imes 10^{-8}$
0.1	AB5	0.36787960	1.8×10^{-7}
	$*F^6$	0.36787960	1.4×10^{-8}

Table 4.3: Performance of our new scheme on second differential equation

True solution for Example 4.3 at x = 1

ster	<u>c</u>	y(x)
0.05	õ	0.36787940
0.12	5	0.36789500
0.1		0.36787950

Note AF5 in the comparison Table 4.3 denote the fifth-order formula due to Abhulimen and Okunuga [3].

Remark 4.5. From the results in Table 4.3, we observed that, our proposed scheme have the least error for various step sizes when compared with the existing methods. We can simply say for now that our new scheme is efficient.

5 Conclusion

From the numerical results presented so far in this paper, it shows that our proposed three-step second derivative exponentially fitted scheme of order six is accurate, efficient and compete favourably with the existing methods which have solve the same set of stiff problems.

In conclusion, our new scheme is A-stable and is appropriate for solving stiff systems whose solutions can be expressed in exponential functions.

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