

**A THREE-STEP SIMPSON'S TYPE
EXPONENTIALLY-FITTED BACKWARD DIFFERENCE
METHOD FOR THE NUMERICAL SOLUTION OF FIRST
ORDER ORDINARY DIFFERENTIAL EQUATIONS**

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ABSTRACT. In this paper, a class of exponential fitting backward difference method (EFBDM) is derived for numerically solving general first order ordinary differential equations. This class of method is from the linear multistep method (LMM) derived via the technique of collocation. The power series polynomial used as basis function is fitted with an exponential function term. This class of EFBDM is derived for the step number $k=3$. The method satisfies the basic features of numerical scheme which includes consistency and zero-stability. The convergence of the method is also established. This class of 3-step method is compared to already existing methods in literature to establish its efficiency in terms of global errors and they compare favourably with the methods cited.

1. INTRODUCTION

In this work, we consider the first order Initial Value Problem (IVP) of the form

$$\left. \begin{aligned} y' &= f(x, y), \quad a < x < b, \\ y(a) &= \alpha_0 \end{aligned} \right\} \quad (1.1)$$

where α_0 is an arbitrary finite real constant, $x \in (a, b)$, $f \in C[a, b]$, is a continuous function defined on the interval (a, b) .

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Several physical processes in science and engineering can be modeled in the form (1.1) which could be non-stiff, stiff or singular in nature. Specifically, we consider non-stiff and singular IVPs that typically originate from models in Mathematical Biology triggered by a random walk of organisms, such as bacterial in the presence of a chemical resulting in interesting spatial patterns (see Tyson *et al.* [18]). We note that the solutions of the non-stiff or singular ODEs may become unbounded in finite time and such a phenomenon is often called blow-up, while the finite time is called the blow-up time (see [19]-[21]).

The idea behind exponential fitting (EF) is to derive numerical methods that are better suited for oscillatory and stiff problems. Classical method with the basis $1, x, x^2, \dots, x^k$ perform best when the solution is a polynomial, as a k -step Adams-Bashforth method can even find a polynomial solution of degree k without errors and up to machine accuracy. The idea of using exponentially fitted formulae for numerically solving differential equations came from Liniger and Willoughby [22], where integration formulae containing free parameters were derived and these parameters were chosen so that the function $\exp(w)$ with w real, satisfied the integration formulae. This was tested on linear and used on multistep method for $k = 1$. From this, many others have developed exponentially-fitted method capable of handling many types of problems especially the nonlinear and oscillatory ones.

To obtain an exponentially fitted variant method, a few of the highest-order monomials are replaced by exponentials. The most general fitting space is of the form $\{1, x, x^2, \dots, x^k, e^{w_0x}, e^{w_1x}, \dots, e^{w_px}\}$ which solely depend on the parameters w_0, \dots, w_p multiplied by the step-size h , see Ixaru and Paternoster [7], Ixaru and Vanden [8]. Particularly, the parameters w_0, \dots, w_p can all be given different values. It can however be interesting to specify a relation between the different parameters. Regardless of the form of the fitting space, it is usually imposed that the parameter value(s) are either real or imaginary, (see [11]-[16]). Here, the exponential fitting space of the form $\{1, x, x^2, x^3, e^{wx}\}$ is used for the derivation of the exponentially fitted method.

2. EXISTENCE AND UNIQUENESS OF FIRST ORDER ODES

The following theorem guarantees the existence of at least one solution of (1.1).

2.1 Existence: Suppose that $f(x, y(x))$ is a continuous function defined in some region

$$R = \{(x, y(x)) : x_0 - \delta < x < x_0 + \delta, y_0 - \varepsilon < y < y_0 + \varepsilon\}$$

containing the point (x_0, y_0) . Then there exists a number $\delta_1 < \delta$ such that a solution $y = f(x)$ of (1.1) is defined for $x_0 - \delta_1 < x < x_0 + \delta_1$,

2.2 Uniqueness: Suppose that both $f(x, y(x))$ and $\frac{\partial f(x, y(x))}{\partial y}$ are continuous functions defined on the region

$$R = \{(x, y(x)) : x_0 - \delta < x < x_0 + \delta, y_0 - \varepsilon < y < y_0 + \varepsilon\}$$

Then there exists a number $\delta_2 < \delta_1$ such that the solution $y = f(x)$ of (1.1) whose existence was guaranteed by the existence theorem, has a unique solution for $x_0 - \delta_2 < x < x_0 + \delta_2$, see Brugnano and Trigiante, [23]-[24].

3. DEVELOPMENT OF THE METHOD

For a 3-step method, we consider the interval $[x_n, x_{n+3}]$, where $x_{n+i} = x_n + ih$, $h = x_j - x_{j-1}$, for solving the problem in (1.1) on the interval $[a, b]$. We consider the approximation of its solution $y(x)$ by a polynomial $u(x)$ given by

$$y(x) \approx u(x) = \sum_{i=0}^3 a_i x^i + a_4 e^{wx} \tag{3.1}$$

whose derivative is given as

$$y'(x) \approx u'(x) = \sum_{i=1}^3 i a_i x^{i-1} + w a_4 e^{wx} \tag{3.2}$$

with the $a_i \in \mathbb{R}$ real unknown parameters to be determined, and the parameter w will be real constant. Imposing appropriate interpolation conditions to $u(x)$ at x_n and collocation condition $u'(x)$ at the points x_n, \dots, x_{n+3} , leads to the system of 4 equations:

$u(x_n) = y_n, u'(x_n + ih) = u'_{n+i} = f_{n+i}; i = 0(1)3$ for the determination of a_i 's, $i = 0(1)3$. Solving the system and obtaining the constants a_0, a_1, a_2, a_3 , which are then substituted into (3.1). The formula of the form

$$u(x) = \alpha_0 y_n + \sum_{i=0}^3 \beta(w; h) f_{n+i} \tag{3.3}$$

is derived, where $\alpha_0 = 1, \beta$ is a function depending on w and h . Evaluating (3.3) at the point $x_{n+i}, i = 0(1)3$, the following 3-step EFBDM are obtained:

$$\begin{aligned}
y_{n+1} &= y_n + \eta_1 \left((12 - 16e^{2hw}hw + 5e^{3hw}hw + e^{hw}(-12 + 23hw))f_n + (-36 + 36e^{hw} - 23hw - 21e^{2hw}hw + 8e^{3hw}hw)f_{n+1} \right. \\
&\quad \left. - (e^{3hw}hw + e^{hw}(36 - 21hw) - 4(9 + 4hw))f_{n+2} + (-12 - 5hw + e^{2hw}hw + e^{hw}(12 - 8hw))f_{n+3} \right) \\
y_{n+2} &= y_n + \eta_2 \left((3 + 7e^{hw}hw + e^{3hw}hw - e^{2hw}(3 + 2hw))f_n + (-9 - 7hw + 4e^{3hw}hw + e^{2hw}(9 - 15hw))f_{n+1} \right. \\
&\quad \left. + (9 - 9e^{2hw} + 2hw + 15e^{hw}hw + e^{3hw}hw)f_{n+2} + (-3 + 3e^{2hw} - hw - 4e^{hw}hw - e^{2hw}hw)f_{n+3} \right) \\
y_{n+3} &= y_n + \eta_1 \left(9(-4 + 4e^{3hw} - 3hw)f_n - (9e^{2hw}hw)f_{n+1} + (9(4 + 9e^{hw}hw + e^{3hw}(-4 + 3hw)))f_{n+2} \right. \\
&\quad \left. + 3(-4 + 4e^{3hw} - 3hw - 9e^{2hw}hw)f_{n+3} \right)
\end{aligned} \tag{3.4}$$

$$\eta_1 = \frac{1}{12w(e^{hw}+1)^3}, \quad \eta_2 = \frac{1}{3w(e^{hw}+1)^3w},$$

3.1. Analysis of the Method.

Local truncation error (LTE) and order

The linear difference operators associated with the formulas in (3.4), is given as

$$\mathcal{L}_k[y(x); h] \equiv y(x + nh) - y(x) - \left[\sum_{i=1}^3 \beta_i(w; h)y'(x + ih) \right] \tag{3.5}$$

The local truncation error of each of the formulae in (3.4) is the amount by which the exact solution of the ODEs fails to satisfy the corresponding difference operator. Thus, if we consider the exact solution $y(x)$ in (3.5), after expanding in Taylor series around x we get that each of the local truncation errors of the form

$$\mathcal{L}[y(x); h] = C_{p+1}h^{p+1}y^{(p+1)}(x) + O(h^{p+2}) \tag{3.6}$$

where the constants C_i for $i = 0(1)p$ vanishes. The C_{p+1} is called the principal error constant and p is called the order of the formula. In this case, for all the formulae in (3.4), the form of (3.6) are given as

$$C_{p+1} = \begin{pmatrix} -\frac{95}{288} \left(wy^{(5)}(x) - y^{(6)}(x) \right) h^6 + O(h)^7 \\ -\frac{14}{45} \left(wy^{(5)}[x] - y^{(6)}(x) \right) h^6 + O(h)^7 \\ -\frac{51}{160} \left(wy^{(5)}[x] - y^{(6)}(x) \right) h^6 + O(h)^7 \end{pmatrix}$$

Conclusively, the order $p = 5$.

3.2. Zero-stability.

Definition 3.2.1: The first characteristic polynomial of k-step linear multistep method is the degree-k polynomial

$$\rho(z) = \sum_{j=0}^k \alpha_j z^j \tag{3.7}$$

Definition 3.2.2: A polynomial is said to satisfy the root condition if all its roots lie within or on the unit circle, with those on the boundary

being simple. In other words, all roots satisfy $|z| \leq 1$ and any that satisfy $|z| = 1$ are simple. A polynomial satisfies the strict root condition if all its roots lie inside the unit circle; that is, $|r| < 1$, Amodio and Mazzia, [1].¹

Definition 3.2.3: A Linear Multistep Method is said to be zero-stable if its first characteristic polynomial $\rho(z)$ satisfies the root condition.

The methods in (3.4) if put the block form can be written as

$$A_0 Y_{r+n} = A_1 Y_r + hB(h; w) F_{r+n} \tag{3.8}$$

The zero-stability is concerned with the stability of the difference system (3.8) as $h \rightarrow 0$. Thus, as $h \rightarrow 0$, (3.8) becomes

$$A_0 Y_{r+n} = A_1 Y_r \tag{3.9}$$

where

$$Y_{r+n} = (y_{n+1}, y_{n+2}, y_{n+3})^T, \quad Y_r = (y_n, y_{n-1}, y_{n-2})^T$$

A_0 is a 3 by 3 identity matrix written as $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ and

$A_1 = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$. Hence we sought for the characteristic polynomial

$$\rho(z) = |zA_0 - A_1| = 0 \tag{3.10}$$

such that the roots $\rho(z) = z^2(z - 1) = 0, z = 1, 0, 0$. Consequently, the method is zero-stable, since the roots of the characteristic polynomial are all zero except one, whose modulus is one (see Dahlquist [3], Lambert [10]). For convergence, we state the following theorem.

3.3. Convergence.

Theorem 3.3.1 Henrici [5]. A linear multistep method is said to be convergent if it is consistent (with order $p \geq 1$) and it is zero-stable.

By the above analysis, the method has order $p > 1$, and is zero-stable. Thus, by the above theorem, the method is convergent.

¹We say that λ is a simple root of $\rho(z)$ if $\lambda - z$ is a factor of $\rho(z)$.

3.4. Implementation of EFBDM.

The block method is implemented as follows: Using method (3.8), $n = 0$, solve for the values of y_1 with the aid of Newton's Method on the sub-interval $[x_0, x_1]$, as y_0 is known from the IVP (1.1). Next, for $n = 1$, the values of y_2 is obtained over the sub-interval $[x_1, x_2]$, as y_1 is known from the previous sub-interval. The process is continued for $n = 2, \dots, N - 1$ to obtain the numerical solution of (1.1) on the sub-intervals $[x_2, x_3], [x_3, x_4], \dots, [x_{N-1}, x_N]$. It should also be noted that the frequency w is determined by the exponential term in the exact solution. Other values can be used in a case where the exact solution is unknown. The details of the implementation is given in Algorithm below.

Algorithm 1 Block Algorithm for EFBDM

1 **begin procedure**ENTER Partitions (a, b, N, h , variables)
 2 For $x_n = x_{n-1} + h, n = 1, \dots, N, h = \frac{b-a}{N}$
 3 Generate block system
 4 Solve [sysytem, variables]
 5 Obtain y_n
 6 **end procedure**

4. NUMERICAL EXAMPLES

In this section, we give numerical examples to illustrate the accuracy of the method. Let $y(x_n)$ be the exact solution and y_n the approximate solution on the partition π_N , we find the absolute errors of the approximate solution as $|y(x_n) - y_n|$

Problem 1. We consider the linear IVP, [2].

$$\begin{cases} y'' = 2, & 0 \leq x \leq 1 \\ y(0) = 1 \end{cases} \quad (4.1)$$

The analytic solution is given by $y(x) = -2 - 2x - x^2 + 3e^x$; With $N = 10, w = -1$.

From the above table, our method become superior over the method in [2].

Problem 2. We consider the singular IVP discussed in [9].

$$\begin{cases} y'' = 1, & 0 \leq x \leq 1 \\ y(0) = 1 \end{cases} \quad (4.2)$$

The analytic solution is given by $y(x) = \tan(x + \frac{\pi}{4})$. With $N = 20$.

TABLE 1. Comparison of absolute errors obtained in different methods for Example 1.

x	y_{app}	y_{ex}	EFBDM	Method in [2]
0.1	1.105512754	1.105512754	1.77E-15	2.45E-5
0.2	1.224208274	1.224208274	1.73E-14	2.71E-5
0.3	1.359576422	1.359576422	7.11E-15	2.99E-5
0.4	1.515474092	1.515474092	2.66E-14	3.31E-5
0.5	1.696163812	1.696163812	4.79E-14	3.65E-5
0.6	1.906356401	1.906356401	1.51E-14	4.04E-5
0.7	2.151258122	2.151258122	7.11E-15	4.46E-5
0.8	2.436622785	2.436622785	3.91E-14	4.93E-5
0.9	2.768809333	2.768809333	6.75E-14	5.45E-5
1.0	3.154845485	3.154845485	8.17E-14	6.03E-5

TABLE 2. Comparison of absolute errors for Example 2.

x	EFBDM	PCM	SSM	RKM
0.0	0	0.00	0.00	0.00
0.1	6.71(-10)	1.06(-6)	1.03(-6)	2.15(-8)
0.2	7.88(-9)	2.71(-6)	2.45(-6)	2.80(-8)
0.3	1.63(-8)	5.37(-6)	4.68(-6)	5.21(-7)
0.4	2.09(-8)	1.03(-5)	8.71(-6)	3.63(-6)
0.5	2.65(-8)	2.13(-5)	1.75(-5)	2.60(-5)
0.6	2.77(-8)	5.54(-5)	4.41(-5)	2.91(-4)
0.7	1.56(-8)	2.80(-4)	2.14(-4)	1.34(-2)
0.8	3.05(-8)	1.02(-2)	7.37(-3)	1.39(-3)
0.9	1.87(-7)	1.58(-4)	1.18(-4)	∞
1.0	7.46(-7)	4.43(-5)	3.22(-5)	∞

NSDM is nonlinear one-step second derivative method with a variable step-size implementation based on continued fractions for the numerical solution of singular initial value problems (IVPs) in [9]. The method was implemented in Predictor-Corrector Mode (PCM) and Self-Starting Mode (SSM). Where RKM is the Runge-Kutta Method for the same problem. It can be clearly seen that our method compares favourably. This shows the superiority of our method.

Problem 3. We consider a linear system of IVP, [17].

$$\begin{pmatrix} y_1'(x) \\ y_2'(x) \end{pmatrix} = \begin{pmatrix} -2y_1(x) + y_2(x) \\ 998y_1(x) - 999y_2(x) \end{pmatrix} + \begin{pmatrix} 2\sin(x) \\ 999(\cos(x) - \sin(x)) \end{pmatrix}, \quad \begin{pmatrix} y_1(0) \\ y_2(0) \end{pmatrix} = \begin{pmatrix} 2 \\ 3 \end{pmatrix} \tag{4.3}$$

TABLE 3. EFBDM absolute errors for Example 3.

x	y_1 Approx	y_1 Exact	y_2 Approx	y_2 Exact	Error 1	Error 2
5.0	-0.9454483808	-0.9454483808	0.2971380792	0.2971380792	2.15E-10	2.17E-10
50.0	-0.26237485419	-0.2623755419	0.9649660279	0.9649660279	4.92E-10	4.97E-10

TABLE 4. Errors for Example 3 in [17]

x	Error 1 of Method 1	Error 2 of Method 1	Error 1 of Method 2	Error 2 of Method 2
5.0	1.27E-3	1.35E-6	1.19E-3	1.26E-6
50.0	3.70E-5	1.10E-7	3.27E-5	1.02E-7

TABLE 5. Maximum errors obtained for Example 4.

Methods	$Max\{y_1, y_2\}$
EFBDM	9.21E-20
BLOCK10SIMP	1.00E-14
BLOCK10	1.00E-15
BLOCK2SIMP	1.00E-6
BLOCK2	1.00E-6

The exact solution is

$$\begin{pmatrix} y_1(x) \\ y_2(x) \end{pmatrix} = \begin{pmatrix} 2e^{-x} + \sin(x) \\ 2e^{-x} - \cos(x) \end{pmatrix} \quad (4.4)$$

Here, $w = 1$.

We remark that EFBDM is very competitive with both methods discussed in [17]. Hence, this shows the superiority of our methods in terms of the errors obtained.

Problem 4. Consider the following system of first order IVP discussed in [6].

$$\begin{aligned} y_1' &= -1002y_1 + 1000y_2^2, & y_1(0) &= 1 \\ y_2'(x) &= y_1 - y_2(1 + y_2), & y_2(0) &= 1 \end{aligned} \quad (4.5)$$

The exact solution are; $y_1(x) = e^{-2x}$, $y_2(x) = e^{-x}$, $w = 2$.

The above Table 5 shows the maximum error of y_1 and y_2 , that is, $Max\{y_1, y_2\}$.

Here, in [6], BLOCK2 is the 2-step block method, BLOCK2SIMP is the simplest 2-step block method, BLOCK10 is the 10-step block method, BLOCK10SIMP is the simplest 10-step block method. The proposed method performed better than the methods compared with in [6].

TABLE 6. Absolute errors for Example 5.

h	Method 1 in [25]	Method 2 in [25]	Method 3 in [25]	EFBDM
10^{-10}	5.20713×10^{-10}	1.02940×10^{-12}	5.06390×10^{-12}	1.24575×10^{-16}
10^{-11}	1.67741×10^{-10}	2.72390×10^{-12}	4.40500×10^{-13}	3.42518×10^{-17}
10^{-12}	5.33553×10^{-11}	1.16940×10^{-12}	2.01000×10^{-14}	4.15785×10^{-17}
10^{-13}	1.68998×10^{-11}	3.96500×10^{-13}	1.40000×10^{-15}	1.27154×10^{-18}

Problem 5. Consider a first order nonlinear singular IVP solved in [6].

$$y' = -\frac{y^2}{\sqrt{x}}, \quad y(0) = 1, \quad 0 < x \leq 1 \tag{4.6}$$

The exact solution is given by $y(x) = \frac{1}{1+2\sqrt{x}}$. We thus solve the initial value problem (4.6) by adopting the same value for the step-size $h = 1/12000000$ as in [6].

Table 6 shows, that for very small h , EFBDM produced excellent results than methods proposed in [25]. It was keenly observed that, even as x is very close to singular 0, the results are not affected. Hence, the proposed EFBDM solved the problem and the results obtained are more superior in terms of the error obtained when compared to the errors obtained in [25].

To show the accuracy of the EFBDM, we solve Susceptible, Exposed, Infective and Recovery (SEIR) tuberculosis disease model in [26] with EFBDM and compare graphically with Runge-Kutta method of order 4.

Problem 6. Consider the SEIR tuberculosis disease model discussed in [26].

$$\begin{aligned} \frac{ds}{dt} &= \mu - \mu s - \beta si \\ \frac{de}{dt} &= \beta si - (\mu + \epsilon)e \\ \frac{di}{dt} &= \epsilon e - (\mu + \gamma)i \\ \frac{dr}{dt} &= \gamma i - \mu r \end{aligned} \tag{4.7}$$

where $s = \frac{S}{N}$, $e = \frac{E}{N}$, $i = \frac{I}{N}$, and $r = \frac{R}{N}$, represents the fractions of the susceptible S , exposed E , infective I and recovery R classes in the population respectively, with initial conditions $s(0) = s_0$, $e(0) = e_0$, $i(0) = i_0$, $r(0) = r_0$. The following are the parameters used for numerical simulation: $s(0) = 5000$, $e(0) = 1000$, $i(0) = 150$, $r(0) = 50$, $\beta = 0.0468$, $\epsilon = 0.1196$, $\gamma = 0.1472$, $\mu = 0.0006$. The figures below show the comparison of EFBDM and the fourth order Runge-Kutta method.

The proposed method was used with appropriate step-size h depending on the method being compared with and the frequency $w = 1$. The

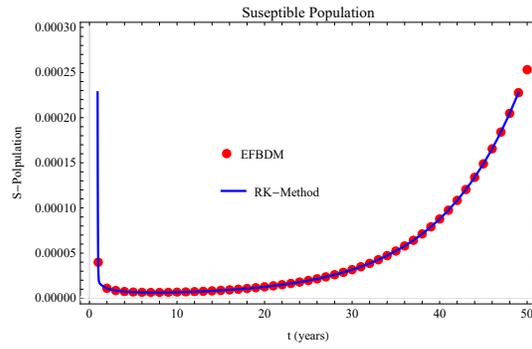


FIGURE 1. Susceptible Population

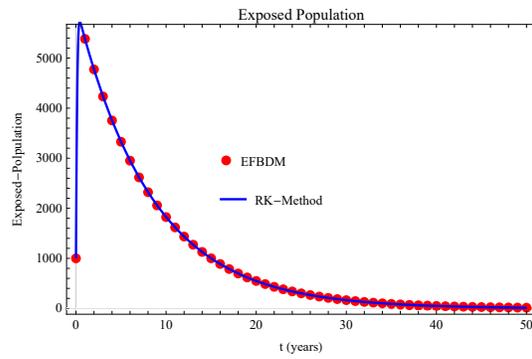


FIGURE 2. Exposed Population

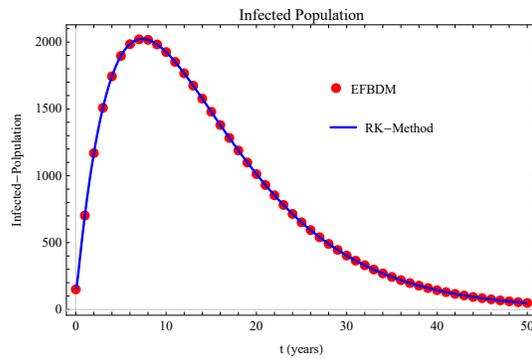


FIGURE 3. Infective Population

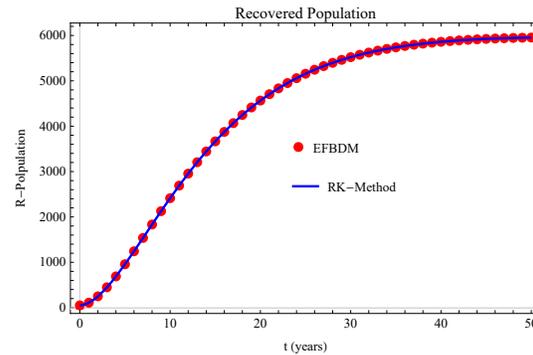


FIGURE 4. Recoverable Population

performance of the EFBDM has been demonstrated to outperform other methods compared with in the cited literature evidently from Problems 1 through 5.

5. CONCLUSION

An Exponentially-fitted Backward Difference Formula (EFBDM) based on continuous linear multistep method is proposed and applied to solve first order linear and non linear IVPs in ordinary differential equations. It can be seen that the method is very easy to derive and less ambiguous. It can be applied to solve a wide range of first order ODEs as seen in the numerical examples. The method shows a very high accuracy when compared to the exact solution and existing methods in the literature.

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