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Exponentially fitted third derivative three-step methods for numerical integration of stiff initial value problems



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ABSTRACT

In this paper, we consider the construction of exponentially fitted third derivative threestep method of order six for the numerical integration of stiff initial-value problems. The numerical analysis of the stability of the new method was discussed and some numerical experiments confirming theoretical expectation are provided. Finally, the numerical results show that the new method is A-stable and compete favorably with the existing methods in terms of efficiency and accuracy.

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1. Introduction

In this paper the author focused on a class of exponentially fitted 3-step third derivative methods suitable for the approximate numerical integration of stiff systems of first order ordinary differential equations of the form.

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

on finite interval $x \in [a, b]$, $y \in R^N$, where the Jacobian arising from (1.1) varies slowly and the eigen-values of J have negative real parts. The problem called the "stiff" are too important to ignore, and too expensive to over power. They are too important to ignore because, they occur in many physically important situations, they are too expensive to overpower because of their size and the inherent difficulty they present to classical methods [13].

However, we will not call a problem stiff unless its solution is slowly varying with respect to the most negative real part of the eigen value.

The spirit behind the development of this kind of numerical integrator is that exponentially fitted formula posse a large region of absolute stability when compared with conventional ones [9].

In the last decade, several authors such as Enright [7], Enright and Pryce [8], Brown [5], Cash [6], Jackson and Kenue [10], Voss [15], Okunuga [12], Abhulimen and Okunuga [1] and Abhulimen and Omeike [3] developed second derivative integrators for the numerical solutions of stiff differential equations. These integrators however were found to be A-stable, particularly for stiff problems whose solutions have exponential functions.

Meanwhile, the aim of this present paper is to derive a class of a three-step third derivative exponential fitting integrators of order six, which is A-stable for all choices of the fitting parameters. The important aspect of these classes of exponentially fitted integrators is that they contain "built-in" local error estimate which may be used as basis of steps control procedure [6].

2. General principle in the derivation of the integrators

In the spirit of [5,1], the general form taken in the derivation of the new integrators considered in this paper is

$$\sum_{i=0}^{k} \alpha_{i} y_{n+i} = h \sum_{i=0}^{k+1} \beta_{i} f_{n+i}^{(1)} + h^{2} \sum_{i=0}^{k} \phi_{i} f_{n+i}^{(2)} + h^{3} \sum_{i=0}^{k} \omega_{i} f_{n+i}^{(3)},$$

$$(2.1)$$

where y_{n+i} is the approximate numerical solution obtained at x_{n+i} and

$$f(x_{n+i},y(x_{n+i}))=y'_{n+i},$$

$$f'(x_{n+i}, y(x_{n+i})) = y''_{n+i},$$

$$f''(x_{n+i}, y(x_{n+i})) = y'''_{n+i}$$

where y'_{n+i} , y''_{n+i} , and y''_{n+i} are the first, second and third derivative of y_{n+i} respectively. So, following the general approach adopted in [6], we use (2.1) as the corrector and the conventional multiderivative multistep formula (2.2) below as a predictor.

$$\sum_{i=0}^{k} \overline{\alpha_{i}} \overline{y}_{n+i} = h \sum_{i=0}^{k} \overline{\beta_{i}} \overline{f}_{n+i}^{(1)} + h^{2} \sum_{i=0}^{k} \overline{\phi_{i}} f_{n+i}^{(2)} + h^{3} \sum_{i=0}^{k} \overline{\omega_{i}} \overline{f}_{n+i}^{(3)}.$$
(2.2)

Meanwhile, the procedure employed in the derivation of the integrator is that both (2.2) and (2.1) contains free parameters.

2.1. Derivation of integrators of order six

To derive a three-step third derivative exponentially scheme, of order six, we first derived the predictor, with $\alpha_k = \alpha_3 = +1$

$$\beta_3 = a$$
 (free parameter).

Here, we deduce six set of simultaneous equation from (2.2), by setting $\alpha_i = \beta_i = \phi_i = 0$, i = 1, 2

$$\overline{\alpha_0} + 1 = 0,$$

$$\overline{\beta_0} + a = 3,$$

$$\overline{\phi_0} + \overline{\phi_3} + 3a = \frac{9}{2},$$

$$3\overline{\phi_3} + \overline{\omega_0} + \overline{\omega_3} + \frac{9}{2}a = \frac{9}{2},$$

$$3\overline{\phi_3} + 2\overline{\omega_0} + 3a = \frac{9}{4},$$

$$4\overline{\phi_3} + 4\overline{\omega_0} + 3a = \frac{9}{5}.$$
(2.3)

When we solve for the unknown parameters we obtain

$$\overline{\alpha_0} = -1$$
, $\overline{\alpha_3} = +1$,

$$\overline{\beta_0} = 3 - a$$
, $\overline{\beta_3} = a$,

$$\overline{\phi_0} = \frac{63}{20} - \frac{3}{2}a, \quad \overline{\phi_3} = \frac{27}{20} - \frac{3}{2}a,$$

$$\overline{\omega_0} = \frac{27}{20} - \frac{3}{4}a = \overline{\omega_3} = \frac{-9}{10} + \frac{3}{4}a.$$

Substituting these values into Eq. (2.2) we obtain the predictor scheme of order six as follows.

$$\overline{y}_{n+3} = y_n + h \left[(3-a)y'_n + ay'_{n+3} \right] + h^2 \left[\left(\frac{63}{20} - \frac{3}{2}a \right) y''_n + \left(\frac{27}{20} - \frac{3}{2}a \right) y''_{n+3} \right] + h^3 \left[\left(\frac{23}{20} - \frac{3}{4}a \right) y'''_n + \left(\frac{-9}{10} + \frac{3}{4}a \right) y'''_{n+3} \right]. \tag{2.4}$$

Next, we introduce the scalar test function for the purpose of the exponential fitting condition of the method as follows.

$$Y' = \lambda y, \quad y_{(0)} = 1.$$
 (2.5)

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