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A note on variable step-size formulation of a Simpson's-type second derivative block method for solving stiff systems

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ABSTRACT

In this paper, a variable step-size formulation of a Simpson's-type second derivative block method is considered as an embedded-type method. This embedded-type method is more effective than its existing fixed step-size counterpart. The numerical experiments considered revealed the superiority of the variable step-size version of the method in comparison with methods of similar characteristics in the literature.

1. Introduction

Our goal is to approximate on a given interval the solution of a first-order initial value problem (IVP) of the form

$$y'(x) = f(x, y(x)), \quad y(a) = y_0 \tag{1}$$

where $x \in [a, b] \subset \mathbb{R}$ and $y(x), f(x, y(x)) \in \mathbb{R}^n$. Although there is a huge amount of step by step methods for solving IVPs, the block methods have been developed in order to obtain the numerical solution at more than one point at a time, looking for computational efficiency. Block methods have been firstly proposed by Milne [1] to be used only as a means of obtaining starting values for predictor–corrector methods. Sarafyan [2] also considered them for similar purposes. Rosser [3] developed Milne's proposals into algorithms for general purpose. For the development and use of block methods for different classes of problems see [1–7]. The block methods contain main and additional formulas, a concept that is due to Brugnano and Trigiante [8]. Some

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advantages of block methods include (i) overcoming the overlapping of pieces of solutions and (ii) that they are self starting, thus avoiding the use of other methods to get starting solutions. According to Hairer et al. [9], to be efficient, a particular algorithm should be suitable for a variable step-size formulation.

In this article, we propose a variable step-size formulation of the existing fixed step-size Simpson's-type second derivative method proposed by Sahi et al. [10]. This method has sixth algebraic order of convergence and is $\mathcal{A}$-stable (a favorable property for solving stiff systems). The existing two-step second derivative method [10] is given by the two formulas

$$\begin{aligned} y_{n+1} &= y_n + \tfrac{h}{240}\left(13hf'_n - 40hf'_{n+1} - 3hf'_{n+2} + 101f_n + 128f_{n+1} + 11f_{n+2}\right) \\ y_{n+2} &= y_n + \tfrac{h}{15}\left(hf'_n - hf'_{n+2} + 7f_n + 16f_{n+1} + 7f_{n+2}\right). \end{aligned} \tag{2}$$

This method simultaneously produces the approximate values of the solution of (1) at two grid points x_{n+1} and x_{n+2}. In the literature, only the constant step-size version of this method is discussed. In virtually, all modern codes for ODEs, the step-size is selected automatically to achieve reliability and efficiency [11]. Practically speaking, any discretization integrator with constant step-size performs poorly if the solution varies rapidly in some parts of the integration interval and slowly in other large parts of the integration interval. Therefore, from a practical point of view, a numerical method must be suitable for variable step-size implementation.

The article is organized as follows: In Section 2, a variable step-size formulation of the block method (2) is presented as an embedded-type method. In Section 3, a pseudo code of this embedded-type method is given. Finally, some numerical experiments have been presented in Section 4 to illustrate the performance of this embedded-type formulation.

2. Formulation in variable step-size mode

The block method in (2) may be formulated in variable step-size mode by considering a lower order method in order to estimate the local error at the final point in each block. For the block method considered, the third order Kutta's method given by

$$\begin{aligned} k_1 &= f(x_n, y_n) \\ k_2 &= f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2}k_1\right) \\ k_3 &= f(x_n + h, y_n - hk_1 + 2hk_2) \\ y_{n+1} &= y_n + \frac{h}{6}(k_1 + 4k_2 + k_3) \end{aligned} \tag{3}$$

has been used to estimate the local error at the final point in each block $[x_n, x_{n+2}]$. This error estimate EST provides the basis for determining the step-size to be used in the next block. In implementation, if the local error is smaller than a given tolerance TOL, the algorithm will change the step-size, from old (h_{old}) to new (h_{new}) as

$$h_{new} = \nu\, h_{old}\left(\frac{TOL}{\|EST\|}\right)^{1/(p+1)}, \tag{4}$$

where p is the order of the lower order method, in this case $p = 3$, and $0 < \nu < 1$ is a safety factor whose purpose is to avoid failed steps.

Normally some restrictions must be considered in order to avoid large fluctuations in step-size: step-size is not allowed to decrease by more than h_{mini} (minimum step-size allowed) or increase by more than h_{maxi} (maximum step-size allowed). This may be included in the implementation using an *If* statement:

$$\textbf{If} \quad h_{mini} \le h_{new} \le h_{maxi} \quad \textbf{then} \quad h_{old} = h_{new}.$$