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DERIVATION OF 2-POINT ZERO STABLENUMERICAL ALGORITHM OF BLOCK BACKWARD DIFFERENTIATION FORMULA FOR SOLVING FIRST ORDER ORDINARY DIFFERENTIAL EQUATIONS

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ABSTRACT
This paper is aimed at deriving a 2-point zero stable numerical algorithm of block backward differentiation formula using Taylor series expansion, for solving first order ordinary differential equation. The order and zero stability of the method are investigated and the derived method is found to be zero stable and of order 3. Hence, the method is suitable for solving first order ordinary differential equation. Implementation of the method has been considered.

Keyword: Block, Backward differentiation formula, Zero stability, Order

INTRODUCTION

Problems in electrical circuits, mechanics, vibrations, chemical reactions, kinetic and population growth can be modeled by differential equations. Such differential equations can be categorized into stiff and non stiff. Majority of both categories cannot be solved analytically and hence the use of suitable numerical schemes is advocated. This paper aimed at driving a two point numerical scheme using Taylor series expansion for the solution of stiff ordinary differential equations. Stiff differential equations describe equations where different physical phenomena acting on different time scales occur simultaneously. Such models brought stiff ordinary differential equations. Block backward differentiation formula is one of the reliable block numerical methods for obtaining solutions of stiff initial value problems. Backward differentiation formula was first discovered by (Curtiss & Hirschfelder, 1952), in his method integration of stiff equations, Cash (1980) extended the work of Curtiss, with integration of stiff system of ODEs using extended backward differentiation formula, Milner (1953) discovered block numerical solution of differential equation, Brugano (1998) with solving differential problem by multistep method, Chu and Hamilton (1987) with parallel solution of ODE's by multistep method, Dalquish (1974) with problem related to numerical method. Implicit methods for solving stiff initial value problem, both methods are zero and A-stable can handle stiff problem with appreciated results. Musa (2012, 2013 & 2014) with a new super class of block backward differentiation formula, an accurate block solver and a new variable step size block method, Musa and Unwala (2019); with Extended 3-point super class of block backward differentiation formula for solving initial value problem. All the methods are both zero and A-stable and performed better in terms of accuracy, maximum error and reduced computational time.

DERIVATION OF THE METHOD

Consider

$$\sum_{j=0}^{3} \alpha_{j,i} y_{n+j-1} = h\beta_{k,1} f_{n+k} \qquad (1)$$

The implicit method in (1) is constructed using a linear operator. To derive the first point y_{n+1}
And define the operator L_1 associated with (1) by

$L_i[y(x),\ \mathrm{h}]$: $\alpha_{0,i}y_{n-1+}\alpha_{1,i}y_n + \alpha_{2,i}y_{n+1} + \alpha_{3,i}y_{n+2} - h\beta_{k,1}f_{n+k} = 0$

Expanding

$y(x_n - h), y(x_n), y(x_n + h), y(x_n + 2h)\ and f(x_n + h)$.Using Taylor series expansion about x_n

Case $k = i = 1$

$$\alpha_{0,1}\ [y(x_n - h) = y_n - hy_n' + \frac{\mathrm{h}^2}{2!}y_n'' + \frac{\mathrm{h}^3}{3!}y_n''' + \cdots]$$
$$\alpha_{1,1}\ [y(x_n) = y_n]$$
$$\alpha_{2,1}\ [y(x_n + h) = y_n - hy_n' + \frac{\mathrm{h}^2}{2!}y_n'' + \frac{\mathrm{h}^3}{3!}y_n''' + \cdots\ ] \qquad (2)$$
$$\alpha_{3,1}[\ y(x_n + 2h) = y_n - 2hy_n' + 4\frac{\mathrm{h}^2}{2!}y_n'' + 8\frac{\mathrm{h}^3}{3!}y_n''' + \cdots\ ]$$
$$h\beta_{1,1}\ [f(x_n + h = y_n' + hy_n'' + \frac{\mathrm{h}^2}{2!}y_n''' + \cdots]$$

Implies

$$\alpha_{0,1} + \alpha_{1,1} + \alpha_{2,1} + \alpha_{3,1} = 0$$

$-\alpha_{0,1} + \alpha_{2,1} + 2\alpha_{3,1} - \beta_{1,1} = 0$
$\frac{1}{2}\alpha_{0,1} + \frac{1}{2}\alpha_{2,1} + 2\alpha_{3,1} - \beta_{1,1} = 0$ (3)
$-\frac{1}{3}\alpha_{0,1} + \frac{1}{6}\alpha_{2,1} + \frac{4}{3}\alpha_{3,1} - \frac{1}{2}\beta_{1,1} = 0$
Normalizing the coefficient of y_{n+1} ($\alpha_{2,1} = 1$).Solving the simultaneous equation. Thus obtained the following values for$\alpha_{j,i`s}$ *and* $\beta_{j,i`s}$.
$\alpha_{2,1} = 1$
$\alpha_{0,1} + \alpha_{1,1} + +\alpha_{3,1} = -1$
$-\alpha_{0,1} + 2\alpha_{3,1} - \beta_{1,1} = -1$
$\frac{1}{2}\alpha_{0,1} + 2\alpha_{3,1} - \beta_{1,1} = -\frac{1}{2}$ (4)
$-\frac{1}{3}\alpha_{0,1} + \frac{4}{3}\alpha_{3,1} - \frac{1}{2}\beta_{1,1} = -\frac{1}{6}$
Solving the equations simultaneously we get
$\alpha_{0,1} = \frac{1}{3}$

$\alpha_{1,1} = -2$
$\alpha_{3,1} = \frac{2}{3}$
$\beta_{1,1} = 2$and $\alpha_{2,1} = 1$
Substituting these values in (2), we have
$\frac{1}{3}y_{n-1} - 2\,y_n + y_{n+1} + \frac{2}{3}\,y_{n+2} - 2f_{n+1} = 0$
$\Rightarrow y_{n+1} = -\frac{1}{3}\,y_{n-1} + 2\,y_n - \frac{2}{3}\,y_{n+2} + 2f_{n+1} = 0$ (5)

$$\alpha_{0,i}\,y(x_n - h) + \alpha_{1,i}\,y(x_n) + \alpha_{2,i}\,y(x_n + h) + \alpha_{3,i}\,y(x_n + 2h) - h\beta_{k,i}f(x_n + h) = 0 \quad (6)$$

Case 2 $\boldsymbol{k = i = 2}$
$\alpha_{0,2}\,y(x_n - h) + \alpha_{1,2}\,y(x_n) + \alpha_{2,2}\,y(x_n + h) + \alpha_{3,2}\,y(x_n + 2h) - h\beta_{2,2}f(x_n + h) = 0$ (7)
Expanding
$y(x_n - h),\ y(x_n),\ y(x_n + h),\ y(x_n + 2h)$ *and* $f(x_n + h)$ in a Taylor series expansion about x_n
We get

$$\alpha_{0,2}[\,y(x_n - h) = y_n - hy_n' + \frac{h^2}{2!}y_n'' + \frac{h^3}{3!}y_n''' + \cdots\,]$$
$$\alpha_{1,2}\,[y(x_n) = y_n]$$

$\alpha_{2,2}\,[y(x_n + h) = y_n + hy_n' + \frac{h^2}{2!}y_n'' + \frac{h^3}{3!}y_n''' + \cdots]$ (8)
$\alpha_{3,2}\,[\,y(x_n + 2h) = y_n + 2hy_n' + \frac{4h^2}{2!}y_n'' + 8\frac{h^3}{3!}y_n''' + \cdots]$
$-h\beta_{2,2}[\,f(x_n + 2h) = y_n' + 2hy_n'' + \frac{4h^2}{2!}y_n''' + \cdots]$
Collecting like terms and re – arrange
$\alpha_{0,2} + \alpha_{1,2} + \alpha_{2,2} + \alpha_{3,2} = 0$
$-\alpha_{0,2} + \alpha_{2,2} + 2\alpha_{3,2} - \beta_{2,2} = 0$
$\frac{1}{2}\alpha_{0,2} + \frac{1}{2}\alpha_{2,2} + 2\alpha_{3,2} - 2\beta_{2,2} = 0$ (9)
$-\frac{1}{6}\alpha_{0,2} + \frac{1}{6}\alpha_{2,2} + \frac{4}{3}\alpha_{3,2} - 2\beta_{2,2} = 0$
Normalizing the coefficient of y_{n+1} ($\alpha_{3,2} = 1$)
$\alpha_{0,2} + \alpha_{1,2} + +\alpha_{2,2} = -1$
$-\alpha_{0,2} + \alpha_{2,2} - \beta_{2,2} = -2$
$\frac{1}{2}\alpha_{0,2} + \frac{1}{2}\,\alpha_{2,2} - 2\beta_{2,2} = -2$
$-\frac{1}{6}\alpha_{0,1} + \frac{1}{6}\alpha_{2,2} - 2\beta_{2,2} = -\frac{4}{3}$
Solving these problem simultaneously we get
$\alpha_{0,2} = -\frac{2}{11}$
$\alpha_{1,2} = \frac{9}{11}$

$\alpha_{2,2} = -\frac{18}{11}$

Substituting the values of $\alpha_{0,2}, \alpha_{1,2}, \alpha_{2,2}, \alpha_{3,2} \& \beta_{2,2}$ in (7) we obtains

$-\frac{2}{11} y_{n-1} + \frac{9}{11} y_n - \frac{18}{11} y_{n+1} + y_{n+2} - \frac{6}{11} f_{n+2} = 0$

$\Rightarrow y_{n+2} = \frac{2}{11} y_{n-1} - \frac{9}{11} y_n + \frac{18}{11} y_{n+1} + \frac{6}{11} f_{n+2}$ (8)

Hence, we have

$\Rightarrow y_{n+1} = -\frac{1}{3} y_{n-1} + 2 y_n + \frac{2}{3} y_{n+2} + 2h f_{n+1}$

$y_{n+2} = \frac{2}{11} y_{n-1} - \frac{9}{11} y_n + \frac{18}{11} y_{n+1} + \frac{6}{11} f_{n+2}$ (9)

Which is Called 2 – Point Numerical algorithmof block backward differentiation formula(2BBDF).

ORDER OF THE METHOD

Definition(1) Order of the method: The order of the block method (1) and its associated linear operator are given by

$$L[y(x); h] = \sum_{j=0}^{3} [C_j y(x + jh)] - h \sum_{j=0}^{3} [D_j y'(x + jh)]$$

Where p is unique integer such that

$E_q = 0, \ q = 0,1, \dots \ p$ and $E_{p+1} \neq 0$, where the E_q are constant Matrices

Defined by:

$E_0 = C_0 + C_1 + \cdots + C_k$

$E_1 = C_1 + 2C_2 + \cdots + kC_k - (D_0 + D_1 + \cdots + D_k)$

$\vdots$

$E_q = \frac{1}{q!}(C_1 + 2^q C_2 + \cdots + k^q C_k) - \frac{1}{(q-1)!}(D_1 + 2^{q-1} D_2 + \cdots + (k)^{q-1} D_k).$

By definition (1) method (9) can be converted into the general matrix form as follows:

$$\sum_{j=0}^{1} C_j^* Y_{m+j-1} = h \sum_{j=0}^{1} D_j^* Y_{m+j-1}, \ (10)$$

Where C_0^*, C_1^*, D_0^* and D_1^* are square matrices defined by

$$C_0^* = \begin{bmatrix} \frac{1}{3} & 0 \\ -\frac{2}{11} & \frac{9}{11} \end{bmatrix}, \quad C_1^* = \begin{bmatrix} 1 & -\frac{2}{3} \\ -\frac{18}{11} & 1 \end{bmatrix} (11)$$

$$D_0^* = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}, \qquad D_1^* = \begin{bmatrix} -2 & 0 \\ 0 & \frac{6}{11} \end{bmatrix} \qquad (12)$$

and Y_{m-1}, Y_m, F_{m-1} and F_m are column vectors defined by

$Y_m = \begin{bmatrix} y_{n+1} \\ y_{n+2} \end{bmatrix}, Y_{m-1} = \begin{bmatrix} y_{n-1} \\ y_n \end{bmatrix}, F_{m-1} = \begin{bmatrix} f_{n-1} \\ f_n \end{bmatrix}, F_m = \begin{bmatrix} f_{n+1} \\ f_{n+2} \end{bmatrix}$ (13)

Thus, equations (12) can be rewritten as

$$\begin{bmatrix} \frac{1}{3} & 0 \\ -\frac{2}{11} & \frac{9}{11} \end{bmatrix} \begin{bmatrix} y_{n-1} \\ y_n \end{bmatrix} + \begin{bmatrix} 1 & -\frac{2}{3} \\ -\frac{18}{11} & 1 \end{bmatrix} \begin{bmatrix} y_{n+1} \\ y_{n+2} \end{bmatrix} = h \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} f_{n-1} \\ f_n \end{bmatrix} + h \begin{bmatrix} -2 & 0 \\ 0 & \frac{6}{11} \end{bmatrix} \begin{bmatrix} f_{n+1} \\ f_{n+2} \end{bmatrix} (14)$$

C_0^*, C_1^*, D_0^* and D_1^* be block matrices defined in (10) as follows:

$C_0^* = [C_{0,} C_1], \quad C_1^* = [C_2, C_3] D_0^* = [D_0, D_1]$ (15)

$D_1^* = [D_2, D_3].$

where

$$C_{0,} = \begin{bmatrix} \frac{1}{3} \\ -\frac{2}{11} \end{bmatrix}, \ C_1 = \begin{bmatrix} 0 \\ \frac{9}{11} \end{bmatrix}, \ C_2 = \begin{bmatrix} 1 \\ -\frac{18}{11} \end{bmatrix}, C_3 = \begin{bmatrix} \frac{2}{3} \\ 1 \end{bmatrix},, \ D_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, D_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, D_2 = \begin{bmatrix} -2 \\ 0 \end{bmatrix}, \ D_3 = \begin{bmatrix} 0 \\ \frac{6}{11} \end{bmatrix}.$$

(16)

we have

$$E_0 = C_0 + C_1 + C_2 + C_3$$
$$= \begin{bmatrix} \frac{1}{3} \\ -\frac{2}{11} \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{9}{11} \end{bmatrix} + \begin{bmatrix} 1 \\ -\frac{18}{11} \end{bmatrix} + \begin{bmatrix} \frac{2}{3} \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (17)$$
$$E_1 = C_1 + 2C_2 + 3C_3 - (D_0 + D_1 + D_2 + D_3)$$
$$= \begin{bmatrix} 0 \\ \frac{9}{11} \end{bmatrix} + 2\begin{bmatrix} 1 \\ -\frac{18}{11} \end{bmatrix} + 3\begin{bmatrix} \frac{2}{3} \\ 1 \end{bmatrix} - \left[\begin{bmatrix} 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \end{bmatrix} + \begin{bmatrix} -2 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{6}{11} \end{bmatrix}\right] = \begin{bmatrix} 0 \\ 0 \end{bmatrix} (18)$$
$$E_2 = \frac{1}{2!}(C_1 + 2^2C_2 + 3^2C_3) - \frac{1}{1!}(D_1 + 2D_2 + 3D_3)$$
$$= \frac{1}{2!}\left[\begin{bmatrix} 0 \\ \frac{9}{11} \end{bmatrix} + 2^2\begin{bmatrix} 1 \\ -\frac{18}{11} \end{bmatrix} + 3^2\begin{bmatrix} \frac{2}{3} \\ 1 \end{bmatrix} - \frac{1}{1!}\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix} + 2\begin{bmatrix} -2 \\ 0 \end{bmatrix} + 3\begin{bmatrix} 0 \\ \frac{6}{11} \end{bmatrix}\right] = \begin{bmatrix} 0 \\ 0 \end{bmatrix}\right] \quad (19)$$
$$E_3 = \frac{1}{3!}(C_1 + 2^3C_2 + 3^3C_3) - \frac{1}{2!}(D_1 + 2^2D_2 + 3^2D_3)$$
$$= \frac{1}{3!}\left[\begin{bmatrix} 0 \\ \frac{9}{11} \end{bmatrix} + 2^3\begin{bmatrix} 1 \\ -\frac{18}{11} \end{bmatrix} + 3^3\begin{bmatrix} \frac{2}{3} \\ 1 \end{bmatrix} - \frac{1}{2!}\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix} + 2^2\begin{bmatrix} -2 \\ 0 \end{bmatrix} + 3^2\begin{bmatrix} 0 \\ \frac{6}{11} \end{bmatrix}\right] = \begin{bmatrix} 0 \\ 0 \end{bmatrix}\right] \quad (20)$$

$$E_4 = \frac{1}{4!}(C_1 + 2^4C_2 + 3^4C_3) - \frac{1}{3!}(D_1 + 2^3D_2 + 3^3D_3)$$
$$= \frac{1}{4!}\left[\begin{bmatrix} 0 \\ \frac{9}{11} \end{bmatrix} + 2^4\begin{bmatrix} 1 \\ -\frac{18}{11} \end{bmatrix} + 3^4\begin{bmatrix} \frac{2}{3} \\ 1 \end{bmatrix} - \frac{1}{3!}\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix} + 2^3\begin{bmatrix} -2 \\ 0 \end{bmatrix} + 3^3\begin{bmatrix} 0 \\ \frac{6}{11} \end{bmatrix}\right] \neq \begin{bmatrix} \frac{21}{2} \\ -\frac{7}{50} \end{bmatrix}\right] (21)$$

Therefore, the method (9) is of order 3, with error constant $E_4 = \begin{bmatrix} \frac{21}{2} \\ -\frac{7}{50} \end{bmatrix}$.

ZERO STABILITY OF THE METHOD

Consider the 2-point new block algorithm super class of block backward differentiation formula below:

$$y_{n+1} = -\frac{1}{3}\, y_{n-1} + 2\, y_n + \frac{2}{3}\, y_{n+2} + 2hf_{n+1}$$
$$y_{n+2} = \frac{2}{11}\, y_{n-1} - \frac{9}{11}\, y_n + \frac{18}{11}\, y_{n+1} + \frac{6}{11} f_{n+2} \quad (22)$$

Definition (2) Zero Stability

A linear Multistep method (9) is said to be zero stable if no root of the first characteristic polynomial has modulus greater than one and that any root with modulus one is simple.

Definition (3) Characteristic polynomial: The characteristic polynomial of the linear multi-step method (9) is defined by

$$\pi(r, \bar{h}) = \rho(\xi) - \bar{h}\sigma(\xi) = 0 (23)$$

Where $\bar{h} = \lambda h$ *and* $\lambda = \frac{\delta f}{\delta y}$

The first and second characteristics polynomial of the method (9) above are defined by

$$\rho(\xi) = \sum_{j=0}^{k} \alpha_j \xi^j \quad (24)$$

and

$$\sigma(\xi) = \sum_{j=0}^{k} \beta_j \xi^j \quad (25)$$

Therefore, the first characteristic polynomial of the method (1) is given by:

$R(t,\bar{h}) = Det(\mathrm{A} * \mathrm{t} - \mathrm{B}) = 0$ (26)

Where Det stands for the determinant. Thus,

$R(t,\bar{h}) = -\frac{1}{11} - 2t - \frac{20\bar{h}}{11} + \frac{23t^2}{11} - \frac{28\bar{h}t^2}{11} + \frac{12\bar{h}^2t^2}{11} = 0$ (27)

By putting $\bar{h}$ = hλ = 0 in (6), we obtain the first characteristic polynomial as:

$R(t,0) = -\frac{1}{11} - 2\mathrm{t} + \frac{23}{11}t^2 = 0$ (28)

Hence, $t = 0.04347826$ or t = 1(29)

Therefore by definition (2), the method (8) is zero Stable.

IMPLEMENTATION OF THE METHOD

In this section we are going to consider the implementation of the 2-point extended super class of block backward differentiation formula.

Defining an absolute error as

Absolute error $= \left| y_{exact}^{(i)} - y_{approximate}^{(i)} \right|$

And the maximum error is given by

$MAXE = \max_{1 \le i \le T} \left(error^{(i)}\right)$

Where T gives the total number of step .

Let $y_{n+1}^{(i+j)}$ denotes the (i+1)th iteration and

$e_{n+1}^{(i+j)} = y_{n+j}^{(i+j)} - y_{n+j}^{(i)}$ j = 1, 2. (30)

Define

$F_1 = y_{n+1} - \frac{2}{3}y_{n+2} - 2hf_{n+1} - \mathcal{E}_1$

$F_2 = y_{n+2} - \frac{18}{11}y_{n+1} - {}_{11}^{6}hf_{n+2} - \mathcal{E}_2$ (31)

Where

$\mathcal{E}_1 = -\frac{1}{3}y_{n-1} + 2y_n$

$\mathcal{E}_2 = \frac{2}{11}y_{n-1} - \frac{9}{11}y_n$ (32)

Newton's iteration can be transform as

$y_{n+1}^{(i+j)} = y_{n+j}^{(i)} - \left[F_i\left(y_{n+j}^{(i)}\right)\right]\left[F_j'(y_{n+j}^{(i)})\right]^{-1}$ (33)

Hence, Newton iteration can be written as

$\left[F_j'(y_{n+j}^{(i)})\right] e_{n+1}^{(i+j)} = -\left[F_i\left(y_{n+j}^{(i)}\right)\right]$ (34)

Equation (30) is equivalent to :

$$\begin{pmatrix} 1 - 4h\frac{\delta f_{n+1}}{\delta y_{n+1}} & \frac{2}{3} \\ -\frac{18}{11} & 1 - \frac{4}{7}h\frac{\delta f_{n+2}}{\delta y_{n+2}} \end{pmatrix}\begin{pmatrix} e_{n+1}^{(i+1)} \\ e_{n+2}^{(i+1)} \end{pmatrix} = \begin{pmatrix} 1 & -\frac{2}{3} \\ \frac{18}{11} & 1 \end{pmatrix}\begin{pmatrix} y_{n+1}^{(i)} \\ y_{n+2}^{(i)} \end{pmatrix} + h\begin{pmatrix} 2 & 0 \\ 0 & \frac{6}{10} \end{pmatrix}\begin{pmatrix} f_{n+1}^{(i)} \\ f_{n+2}^{(i)} \end{pmatrix} + \begin{pmatrix} \mathcal{E}_1 \\ \mathcal{E}_2 \end{pmatrix} \quad (30)$$

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