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THE HYBRID OBRECHKOFF BDF METHODS FOR THE NUMERICAL SOLUTION OF FIRST ORDER INITIAL VALUE PROBLEMS

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Abstract. In this paper, we introduce the new class of high order hybrid Obrechkoff methods based on backward differentiation formula (BDF), we say HOBDF, for the numerical solutions of first order initial value problems. The numerical results obtained by the new method for some problems show its superiority in efficiency, accuracy and stability.

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1. Introduction

Consider the initial value problem for a single first order ordinary differential equation

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

Initial value problems occur frequently in applications. Numerical solution of these problems is a central task in all simulation environments for mechanical, electrical, chemical systems. There are special purpose simulation programs for application in these fields, which often require from their users a deep understanding of the basic properties of the underlying numerical methods [7, 9, 1, 13, 8]. Kopal, in 1955, believed [12] that extrapolation and substitution methods can be regarded as two extreme ways for the construction of numerical solutions of ordinary differential equations leaving a vast no man's land in between, the exploration of which has barely as yet begun. In this context extrapolation methods means method of linear multistep type and substitution methods means method of Runge-Kutta type.

One of the most important properties for the numerical solution of general first-order differential equations, is lies in satisfying the essential condition of zero-stability. This zero-stability barrier was circumvented by the introduction, in 1964-5, of modified linear multistep formula which incorporate a function evaluation at off-step point. Such formula, simultaneously proposed by Gragg and Stetter [8], Butcher [1] and Gear [7] were christened *hybrid* by the last author an apt name since, whilst retaining certain linear multistep characteristics, hybrid methods share with Runge-Kutta methods the property of utilizing data at points other than the step points. Thus, we may regard the introduction of hybrid formulae as an important step into the no man's land described by Kopal. Several authors and researchers are focusing on the development of more efficient methods, e.g. general linear methods and general multistep methods [9, 11, 14, 16]. We note that the above mentioned methods can be considered as special cases of general linear methods. Most of the improvements in the class of general multistep methods, methods like extended BDF (EBDF), modified EBDF (MEBDF) and adaptive EBDF (A-EBDF) [2, 3, 4, 5] are based on backward differentiation formula (BDF), because of its special properties. These methods are A-stable or A(α)-stable. The first modification introduced by cash [3] was the EBDF in which one superior point has been applied.

In this paper, methods with one stage point (or off-step point), and therefore with one stage equation, are presented which can be considered as a subclass of general multistep methods. Only one off-step point is used in the first and high derivatives $f(x, y)$ of the solution $y(x)$ to improve the absolute stability regions.

2. Main Results

For the numerical integration of (1), we consider k-step HOBDF methods of the form

$$\overline{y}_{n+s} = h\mu f_{n+1} + \sum_{j=0}^{k} \gamma_{n+1-j} y_{n+1-j}, \tag{2}$$

$$\sum_{j=1}^{k} \frac{1}{j} \nabla^j y_{n+1} = h f_{n+1} + h^{k+1} \beta \bar{f}_{n+s}^{(k)}, \tag{3}$$

where

$$f_{n+1} = f(x_{n+1}, y_{n+1}), \quad \bar{f}_{n+s} = f(x_{n+s}, \bar{y}_{n+s}), \quad x_{n+s} = x_n + sh,$$

and γ_i, β and $s \in (0, n)$, and $s \notin \{1, 2, \ldots, n-1\}$, are arbitrary parameters. From (2), it is clear that the order of this hybrid scheme is k where $k = 1, 2, \cdots$. Now with the difference equation (3), we can associate the difference operator L defined next.

Definition 1. *Let the differential equation (1) have a unique solution $y(x)$ on $[a, b]$ and suppose that $y(x) \in C^{(p+1)}[a, b]$ for $p \geq 1$. Then the difference operator L for method (3) can be written as*

$$\begin{aligned} L[y(x), h] &= \sum_{j=1}^{k} \frac{1}{j} \nabla^j y(x+h) - hy'(x+h) \\ &- h^{k+1} \beta \bar{y}^{(k+1)}(x_n + sh). \end{aligned} \tag{4}$$

In order that the difference equation (4) be useful for numerical integration, it is necessary that it be satisfied to high accuracy by the solution of the differential equation $y' = f(x, y)$, when h is small for an arbitrary function $f(x, y)$. This imposes restrictions on the coefficients β and s.

For $k = 2$, we have

$$\begin{aligned} LTE &= -\left[\frac{1}{3} + \beta\right] h^3 y^{(3)}(x) - \left[\frac{1}{12} + \beta s\right] h^4 y^{(4)}(x) \\ &- \left[\frac{1}{30} + \beta\left(s - \frac{1}{2}\right)\right] h^5 y^{(5)}(x) + O\left(h^6\right). \end{aligned} \tag{5}$$

Therefore if we take $\beta = -\frac{1}{3}$ and $s = \frac{1}{4}$, we have

$$\frac{3}{2} y_{n+1} - 2y_n + \frac{1}{2} y_{n-1} = hf_{n+1} - \frac{h^3}{3} \bar{f}''_{n+\frac{1}{4}}, \tag{6}$$

and

$$\bar{y}_{n+\frac{1}{4}} = y_{n+1} - \frac{3h}{4} f_{n+1},$$

which is the two-step hybrid Obrechkoff BDF method of order 4 and its local truncation error is $lte_2 = -\frac{7}{60} h^5 y^{(5)}(x)$.

For $k = 3$, we have

$$\begin{aligned} LTE &= -\left[\frac{1}{4} + \beta\right] h^4 y^{(4)}(x) - \left[as - \frac{1}{20}\right] h^5 y^{(5)}(x) \\ &- \left[\frac{1}{30} + \beta\left(\frac{1}{2} + (s-1) + \frac{1}{2}(s-1)^2\right)\right] h^6 y^{(6)}(x) + O\left(h^7\right). \end{aligned} \tag{7}$$

Therefore if we take $\beta = -\frac{1}{4}$ and $s = -\frac{1}{5}$, we have

$$\frac{11}{6} y_{n+1} - 3y_n + \frac{3}{2} y_{n-1} - \frac{1}{3} y_{n-2} = hf_{n+1} - \frac{h^4}{4} \bar{f}^{(3)}_{n-\frac{1}{5}}, \tag{8}$$

and

$$\overline{y}_{n-\frac{1}{5}} = -\frac{11}{25}y_{n+1} + \frac{6h}{25}f_{n+1} + \frac{36}{25}y_n,$$

which is the two-step hybrid Obrechkoff BDF method of order 5 and its local truncation error is $lte_3 = -\frac{17}{600}h^5y^{(6)}(x)$. Similarly, the all values of s, β and orders of tne new HOBDF method for various k, are shown in Table 1.

3. Order of the truncation error

As mentioned in previous section, the the order of stage (2) and (3) are $k+1$ and $k+2$ respectively. Now, we are going to prove that the new method (2-3) is of order $k+2$, $k = 2, 3, \cdots, 12$. We assume that $y(x)$ be as a solution of (1) with desired continues derivatives. Then the local truncation error for (2) of order $k+1$ is

$$y(x_{n+s}) - \overline{y}_{n+s} = C'h^{k+2}y^{(k+2)}(x_n) + O(h^{k+3}), \tag{9}$$

where $x_{n+s} = x_n + sh$, $s \notin \{0, 1, 2, \ldots, k\}$, and C' is the error constant when the method is being used to get $\overline{y}(x_{n+s})$. Similarly, the local truncation error for method (3) of order $k+2$ is

$$y(x_{n+1}) - y_{n+1} = Ch^{k+3}y^{(k+3)}(x_n) + O(h^{k+4}), \tag{10}$$

where C is the error constant of the method (3). Thus, the following theorem can be obtained.

Theorem 1. *Assume that*
1- formula (2) is of order $k+1$,
2- formula (3) is of order $k+2$,
then, the method (2-3) has order $k+2$.

Proof. Assuming that y_{n+1j}, $j = 1, 2, \cdots, k$, be exact, then from (3) and (10) the difference operator associated with method (3) is

$$\begin{aligned} y(x_{n+1}) - y_{n+1} &= Ch^{k+3}y^{(k+3)}(x_n) \\ &+ h\left[f(x_{n+s}, y(x_{n+s})) - f(x_{n+s}, \overline{y}_{n+s})\right] \\ &+ h^{k+1}\left[f^{(k)}(x_{n+s}, y(x_{n+s})) - f^{(k)}(x_{n+s}, \overline{y}_{n+s})\right] \\ &+O\left(h^{k+4}\right). \end{aligned} \tag{11}$$

For some η_{n+s} in the interval whose end points are $\overline{y}_{n+s}$ and $y(x_{n+s})$, we can write

$$f^{(k)}(x_{n+s}, y(x_{n+s})) - f^{(k)}(x_{n+s}, \overline{y}_{n+s}) = \frac{\partial f^{(k)}}{\partial y}(x_{n+s}, \eta_{n+s})\left(y(x_{n+s}) - \overline{y}_{n+s}\right). \tag{12}$$

Now, from (9-12) we have

$$\begin{aligned} y(x_{n+1}) - y_{n+1} &= h^{k+1}\frac{\partial f^{(k)}}{\partial y}(x_{n+s},\eta_{n+s})\left(y(x_{n+s}) - \overline{y}_{n+s}\right) \\ &\quad + Ch^{k+3}y^{(k+3)}(x_n) + O\left(h^{k+4}\right) \\ &= h^{k+1}\frac{\partial f^{(k)}}{\partial y}(x_{n+s},\eta_{n+s})\left[C'h^{k+2}y^{(k+2)}(x_n) + o\left(h^{k+3}\right)\right] \\ &\quad + Ch^{k+3}y^{(k+3)}(x_n) + O\left(h^{k+4}\right) \\ &= h^{k+3}\left[\frac{\partial f^{(k)}}{\partial y}(x_{n+s},\eta_{n+s})C'y^{(k+2)}(x_n) + Cy^{(k+3)}(x_n)\right] \\ &\quad + O\left(h^{k+4}\right). \end{aligned} \tag{13}$$

It results from the above that the order of new method (2-3) is $k+2$ for $k = 2, 3, \ldots, 12$.

4. Stability analysis

Consider the Dahlquist's test equation of form

$$y' = \lambda y, \qquad y(0) = y_0. \tag{14}$$

Applying method (2-3) to this test equation results in getting equations of the form

$$y_{n+s} = \mu\overline{h}y_{n+1} + \sum_{j=0}^{k}\gamma_{n+1-j}y_{n+1-j}, \tag{15}$$

$$\sum_{j=1}^{k}\frac{1}{j}\nabla^j y_{n+1} = \overline{h}y_{n+1} + h^{k+1}\beta y_{n+s}, \tag{16}$$

where $\overline{h} = h\lambda$. Now, we substitute (15) into (16) and therefore we have

$$\sum_{j=1}^{k}\frac{1}{j}\nabla^j y_{n+1} = \overline{h}y_{n+1} + h^{k+1}\beta\left[\mu\overline{h}y_{n+1} + \sum_{j=0}^{k}\gamma_{n+1-j}y_{n+1-j}\right],$$

hence

$$\sum_{j=1}^{k}\frac{1}{j}\nabla^j y_{n+1} = \overline{h}y_{n+1} + \beta\mu\overline{h}^{k+2}y_{n+1} + \overline{h}^{k+1}\beta\sum_{j=0}^{k}\gamma_{n+1-j}y_{n+1-j}.$$

β	$-\frac{1}{3}$	$-\frac{1}{4}$	$-\frac{1}{5}$	$-\frac{1}{6}$	$-\frac{1}{7}$	$-\frac{1}{8}$	$-\frac{1}{9}$	$-\frac{1}{10}$	$-\frac{1}{11}$	$-\frac{1}{12}$	$-\frac{1}{13}$
k	2	3	4	5	6	7	8	9	10	11	12
Order	4	5	6	7	8	9	10	11	12	13	14
s	$\frac{1}{4}$	$-\frac{1}{5}$	$-\frac{2}{3}$	$-\frac{8}{7}$	$-\frac{13}{8}$	$-\frac{19}{9}$	$-\frac{13}{5}$	$-\frac{34}{11}$	$-\frac{43}{12}$	$-\frac{53}{13}$	$-\frac{32}{7}$

Table 1: The values of s, β and order for HOBDF method.

By setting $y_{n+1-j} = r^{n+1-j}$, the corresponding characteristic equation of the $k+2$th order difference equation of our new HOBDF method is

$$\sum_{j=1}^{k} \frac{1}{j} \nabla^j r^{n+1} = \overline{h} r^{n+1} + \beta\mu \overline{h}^{k+2} r^{n+1} + \overline{h}^{k+1} \beta \sum_{j=0}^{k} \gamma_{n+1-j} r^{n+1-j},$$

and dividing by r^n, we can write

$$\sum_{j=1}^{k} \frac{1}{j} \nabla^j r^{1-j} = \overline{h} r + \beta\mu \overline{h}^{k+2} r + \overline{h}^{k+1} \beta \sum_{j=0}^{k} \gamma_{n+1-j} r^{1-j}.$$

Then we have

$$A\overline{h}^{k+2} + B\overline{h}^{k+1} + C\overline{h} + D = 0, \tag{17}$$

where

$$A = \beta\mu r, \qquad B = \beta \sum_{j=0}^{k} \gamma_{n+1-j} r^{1-j}, \qquad C = r, \qquad D = -\sum_{j=1}^{k} \frac{1}{j} \nabla^j r^{1-j}.$$

To see the zero-stability of this new method, one can easily show that by substituting $\overline{h} = \lambda h = 0$ in (17), the resulting characteristic polynomial satisfies the root condition and so the method is zero-stable. If in (17), we put $\overline{h} = \lambda h$, then one can see that by theorem of Schur [13], the root condition is satisfied by HOBDF. Now, we are going to obtain the absolute stability regions (A(α)-stability) of our presented methods in this paper. For do that, we used the boundary locus method for A(α)-stability of HOBDF. By setting $r = e^{i\theta}$ and then by using (17) obtained $k+2$ roots $\overline{h}_i(\theta)$, $i = 1, 2, \ldots, k+2$, which can give us the stability region of HOBDF. The values of s, β and order for HOBDF method are given in Tables 1. The maximum values of α for BDF, EBDF and MEBDF methods are given in Table 2. The maximum values of α for HOBDF and HBDF methods are given in Table 3.

k	1	2	3	4	5	6	7
BDF							
Order	1	2	3	4	5	6	-
α	90°	90°	88°	73°	51°	18°	-
EBDF							
Order	2	3	4	5	6	7	8
α	90°	90°	90°	87.61°	80.2°	67.7°	48.8°
MEBDF							
Order	2	3	4	5	6	7	8
α	90°	90°	90°	88.4°	82.5°	74.5°	62°
MEBDF							
Order	2	3	4	5	6	7	8
α	90°	90°	90°	88.85°	84.2°	75°	61°

Table 2: A(α)-stability for BDF, EBDF, MEBDF and A-EBDF.

k	1	2	3	4	5	6	7	8	9
HBDF									
Order	-	2	3	4	5	6	7	8	9
α	90°	90°	90°	90°	89.77°	88.46°	85.97°	82.42°	77.75°
HOBDF									
Order	3	4	5	6	7	8	9	10	11
α	90°	90°	90°	90°	89.93°	89.32°	87.67°	85.23°	82.16°

k	10	11	12
HBDF			
Order	10	11	12
α	70.18°	58.96°	46.12°
HOBDF			
Order	12	13	14
α	76.25°	66.84°	58.49°

Table 3: A(α)-stability for HBDF and HOBDF.

N	HOBDF ($k=7$)	HBDF($k=7$)
40	2.37e-18	7.77e-16
	3.21e-38	1.48e-36
	9.64e-39	7.29e-37

Table 4: Comparison of the absolute errors in the approximations using the new method ($k=7$) and HBDF($k=7$) [6] for problem 3.1.

5. Numerical Examples

In this section, we present some numerical results of our new HOBDF method and compare them with that of HBDF method [6].

Example 1. *Consider the initial value problem*

$$\begin{cases} y_1' = -0.1y_1 - 49.9y_2, \\ y_2' = -50y_2, \\ y_3' = 70y_2 - 120y_3, \\ y_1(0) = 2, \quad y_2(0) = 1 \quad y_3(0) = 2. \end{cases}$$

The theoretical solution is

$$\begin{cases} y_1 = e^{-0.1t} + e^{-50t}, \\ y_2 = e^{-50t}, \\ y_3 = e^{-50t} + e^{-120t}. \end{cases}$$

The absolute errors are listed in table 4 for comparison with the HBDF method ($k=7$) [6] and our new HOBDF method ($k=7$).

Example 2. *Consider the stiff initial value problem*

$$\begin{cases} y_1' = -ay_1 - by_2 + (a+b-1)\exp(-x), & y_1(0) = 1, \\ y_2' = by_1 - ay_2 + (a-b-1)\exp(-x), & y_2(0) = 1, \end{cases}$$

with theoretical solution $y_1(x) = y_2(x) = \exp(-x)$. Numerical results have been calculated by $a = 1$ and $b = 30$ in the interval [0,2] are listed in table 5 for comparison with the HBDF method ($k=7$) [6] and our new HOBDF method ($k=7$).

Example 3. *Consider the stiff initial value problem*

$$\begin{cases} y_1' = -1002y_1 - 1000y_2^2, \\ y_2' = y_1 - y_2(1+y_2), \\ y_1(0) = 1, \quad y_2(0) = 1. \end{cases}$$

N	HOBDF ($k = 7$)	HBDF($k = 7$)
20	3.25e-16	2.16e-14
	6.19e-17	5.52e-15
10^2	4.69e-19	2.77e-17
	7.31e-19	5.55e-17
10^3	2.16e-19	2.77e-17
	2.28e-19	2.77e-17

Table 5: Comparison of the absolute errors in the approximations using the new method ($k = 7$) and HBDF($k = 7$) [6] for problem 3.2.

N	HOBDF ($k = 7$)	HBDF($k = 7$)
300	4.21e-15	1.50e-13
	6.31e-13	6.40e-11
800	5.29e-16	1.30e-14
	6.46e-13	1.72e-12
10^4	2.27e-23	4.06e-20
	8.26e-21	8.67e-18

Table 6: Comparison of the absolute errors in the approximations using the new method ($k = 7$) and HBDF($k = 7$) [6] for problem 3.3.

The exact solution is

$$\begin{cases} y_1 = \exp(-2t), \\ y_2 = \exp(-t). \end{cases}$$

The absolute errors are listed in table 6 for comparison with the HBDF method ($k = 7$) [6] and our new HOBDF method ($k = 7$).

Example 4. *Consider the stiff problem*

$$\begin{cases} y_1' = -0.013y_1 - 1000y_1y_2 - 2500y_1y_3, \\ y_2' = -0.013y_1 - 1000y_1y_2, \\ y_3' = -2500y_1y_3, \\ y_1(0) = 0, \quad y_2(0) = 1, \quad y_3(0) = 1. \end{cases}$$

This is a stiff system which has arisen from chemistry problem with initial value $Y(0) = [0, 1, 1]^T$. For details see [10]. We have solved this example in the interval $[0, 2]$ and compared with the exact solutions $y_1 = -0.3616933169289e - 5$, $y_2 = 0.9815029948230$, $y_3 = 1.018493388244$. The numerical results are shown in Table 7

N	HOBDF ($k = 7$)	HBDF($k = 7$)
500	2.37e-16	3.98e-14
	3.21e-12	7.62e-09
	4.64e-12	7.62e-09
5000	2.37e-21	2.54e-19
	4.31e-18	3.00e-15
	8.56e-16	1.72e-13

Table 7: Comparison of the absolute errors in the approximations using the new method ($k = 7$) and HBDF($k = 7$) [6] for problem 3.4.

Conclusion

The absolute stability regions of the HOBDF are larger than those of HBDF, BDF, EBDF, A-EBDF, MEBDF methods, and, these new methods are often superior when high accuracy is requested. The second point is that, it is clear that there is not A(α)-stable BDF method of order more than 6 to compare with HOBDF of order 12. Thus, it can be concluded that our new methods (HOBDFs), based on an additional off-step point, have good stability properties and numerical testing shows good performance comparing with existing BDF, EBDF, MEBDF and HBDF.

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