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Block Method for Generalised Multistep Adams and Backward Differentiation Formulae In Solving First Order ODEs

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Abstract The performance of the Block Generalised Multistep Adams and Backward Differentiation Formulae (BGMBDF) as compared with Generalised Multistep Adams and Backward Differentiation Formulae (GMBDF) is presented. These methods are used to solve initial value problems (IVPs) for stiff and nonstiff systems of ordinary differential equations (ODEs). The results obtained show that the BGMBDF reduces the total number of steps in computation.

Keywords Block, backward differentiation formulae, steps.

1 Introduction to Block Methods

A block method is understood to be a method that computes concurrently solution values at different points on the x-axis. The block method to be developed and analyzed in this paper is based on the idea of simultaneously producing a "block" of approximations $y_{n+1}, y_{n+2}, y_{n+3,.....,}y_{n+k}$. Hence given the previous $(y_{n-1}, y_n)^t$ we modified the algorithm by Suleiman [14] to include the next block $(y_{n+1}, y_{n+2})^t$ in its iteration scheme. This approach was developed by a number of researchers such as Shampine and Watts [12], Butcher[3], Chu and Hamilton [4], Fatunla [5], D.Voss and S.Abbas[15]. In a related study, Omar[10] had considered block method for the solution of nonstiff problem. First, we introduce the basic definition of a block method described by [4].

Definition 1.1

Let Y_m and F_m be vectors defined by

$$Y_m = [y_n, y_{n+1}, y_{n+2}, ..., y_{n+r-1}]^t, \quad (1)$$

$$F_m = [f_n, f_{n+1}, f_{n+2}, ..., f_{n+r-1}]^t. \quad (2)$$

Then a general k-block, r-point method is a matrix of finite difference equation of the form

$$Y_m = \sum_{i=1}^{k} A_i Y_{m-i} + h \sum_{i=0}^{k} B_i F_{m-i} \tag{3}$$

where all the A_i's and B_i's are properly chosen $r \times r$ matrix coefficients and $m = 0, 1, 2, ...$ represents the block number, $n = mr$ the first step number in the m-th block and r is the proposed block size.

2 Block Generalised Multistep Adams and Backward Differentiation Formulae

In this section, we briefly describe the Generalised Multistep Adams and Backward Differentiation Formulae. A GMBDF uses a family of BDF, in variable order, variable step to numerically solve stiff IVPs. We consider BDF methods for the numerical solution of systems of first order ODEs of the form

$$y_i' = f_i\left(x, \tilde{Y}\right), i = 1, 2, ..., s, \tag{4}$$

given initial values $\tilde{Y}(a) = \eta$, where $\tilde{Y}^T(x) = (y_1, y_2, ..., y_s)$ and $\tilde{\eta}^T(x) = (\eta_1, \eta_2, ..., \eta_s)$. Our aim is to produce a block backward differentiation method for the numerical solution of the first order IVP of the form

$$y' = f(x, y), y(a) = \eta, a \le x \le b \tag{5}$$

where η is a given initial value at the initial point $x = a$ and f is continuous and satisfies a Lipschitz condition on the region $[a, b] \times (-\infty, \infty)$. Let y_n and $y(x_n)$ be the computed approximation and the exact solution respectively to (5) at point x_n.

The family of BDF used can be represented by implicit multistep formulas of the form

$$\sum_{i=0}^{q} \left(\alpha_{n,i} y_{n-i} + h_n \beta_{n,i} f(x_n, y_n)\right) = 0 \tag{6}$$

and the coefficients $\alpha_{n,i}$ and $\beta_{n,i}$ are determined by an integration formula.

Definition 2.1

Define the interpolating polynomial $P_{k,n}(x)$ which interpolates the values $f_n, f_{n-1}, ..., f_{n-k}$ of a function f at the points $x_n, x_{n-1}, ..., x_{n-k}$ in terms of k-th divided differences denoted by $f_{[n,n-1,...,n-i]}$ as follows

$$P_{k,n}(x) = f_n + (x - x_n) f_{[n,n-1]} + ..., (x - x_n) ... (x - x_{n-k+2}) f_{[n,n-1,...,n-k+1]}, \tag{7}$$

and

$$f_{[n,n-1,...,n-i]} = \frac{f_{[n,n-1,...,n-i+1]} - f_{[n-1,n-2,...,n-i]}}{x_n - x_{n-i}}.$$

Definition 2.2

Define the integration coefficients $g_{i,t}$, $t > 0$ to be the t-fold integral

$$g_{i,t} = \int_{x_n}^{x_{n+1}} \int_{x_n}^{x} ... \int_{x_n}^{x} P_{n,i}(x)\, dx$$

and

$$g_{i,0} = P_{n,i}(x_{n+1}).$$

Definition 2.3

Define the differentiation coefficients $d_{i,t}$, $t > 0$ by

$$d_{i,t} = \frac{d^t}{dx^t} P_{n,i}(x) \bigg|_{x=x_{n+1}}.$$

Both the integration and the differentiation coefficients can be generated by simple recurrence relation which were derived in Suleiman [14].

The predictor formulae is constructed by first integrating (5) . This leads to

$$y(x_{n+d}) = y(x_n) + \int_{x_n}^{x_{n+d}} f\left(x, \tilde{Y}(x)\right) dx \tag{8}$$

Replace (8) using (7)

$$y_{n+d} = y_n + \int_{x_n}^{x} P_{k,n}(x)\, dx \tag{9}$$

It follows that the predictor formulae are given by

$$\begin{aligned} P_{n+d} &= y_n + \sum_{i=0}^{k-1} g_{i,1} f_{[n,n-1,\dots,n-i]} \\ P'_{n+d} &= \sum_{i=0}^{k-1} g_{i,0} f_{[n,n-1,\dots,n-i]} \end{aligned} \tag{10}$$

The corrector formulae are constructed to provide values that satisfy

$$y' = f(x_{n+d}, y_{n+d}). \tag{11}$$

The corrected values are given by

$$\begin{aligned} {}^1y_{n+d} &= P_{n+d} + \frac{g_{k,t}^{(d)}}{g_{k,0}^{(d)}} e_d \\ {}^1y'_{n+d} &= P'_{n+d} + e_d \end{aligned} \tag{12}$$

where $e_d = f\left(x_{n+d}, \tilde{P}_{n+d}\right) - P'_{n+d}$ and ${}^1y_{n+d}$ denote the first iterative value of y_{n+d}.

In accordance with the terminology used in the linear multistep case, the evaluation was done in PECE mode. P and C indicate one application of the predictor or the corrector respectively, and E indicates one evaluation of the function f, given x and y. PECE modes for block methods described by [4] is defined as follows:

$$
\begin{aligned}
P:&\quad \begin{aligned} P_{n+d} &= y_n + \sum_{i=0}^{k-1} g_{i,1} f_{[n,n-1,\ldots,n-i]} \\ P'_{n+d} &= \sum_{i=0}^{k-1} g_{i,0} f_{[n,n-1,\ldots,n-i]} \end{aligned} \\
E:&\quad {}^1y' = f\left(x_{n+d}, {}^0y_{n+d}\right), \quad \text{where} \quad {}^0y_{n+d} = P_{n+d} \\
C:&\quad \begin{aligned} {}^1y_{n+d} &= P_{n+d} + \frac{g_{k,t}^{(d)}}{g_{k,0}^{(d)}} e_d \\ {}^1y'_{n+d} &= P'_{n+d} + e_d \end{aligned} \\
E:&\quad y'_{n+d} = f\left(x_{n+d}, {}^1y_{n+d}\right)
\end{aligned}
$$

The simultaneous sequence of computation for the first point in the block BDF is

$$\rightarrow y_{n+1}^p \rightarrow f_{n+1}^p \rightarrow y_{n+1}^c \rightarrow f_{n+1}^c$$

and the computation for the second point is

$$\rightarrow y_{n+2}^p \rightarrow f_{n+2}^p \rightarrow y_{n+2}^c \rightarrow f_{n+2}^c.$$

3 Numerical Results

The numerical method described in the previous sections was applied to six problems from the literature. Each problem is defined by a differential equation and an error tolerance. The existing code INTEGRATE2 by Suleiman [14] was modified and redesigned to include the new block algorithm in its iteration scheme.

Test Problems

These problems were solved numerically using the BGMBDF and GMBDF of variable step size and order using three different tolerances $10^{-2}, 10^{-4}$ and 10^{-6}.

For the numerical results we recorded the following quantities:

Tol	:	The upper bound for the local error estimate
N_{reject}	:	The total number of rejected steps due to convergence failure or local error control
$N_{success}$	:	The total number of accepted steps
N_{total}	:	The total number of steps to the integration
Max_{error}	:	Maximum error
$Step_r$	:	Percentage total step reduction

In Table 3.1–3.6 we present the performance measures such as the number of success steps, number of fail steps, the maximum error and the total number of steps taken. Note that the BGMBDF requires less number of steps compared to the GMBDF method.

Problem	Differential equation	Initial values	Range of integration	Source
1.	$y' = -0.5y$ Exact solution: $y(x) = e^{-0.5x}$	$y(0) = 1$	$0 \le x \le 20$	Burden[2]
2.	$y' = -y$ Exact solution: $y(x) = e^{-x}$	$y(0) = 1$	$0 \le x \le 20$	Birta [1]
3.	$y' = -30y$ Exact solution: $y(x) = e^{-30x}$	$y(0) = 1$	$0 \le x \le 20$	Burden[2]
4.	$y' = -300xy$ Exact solution: $y(x) = e^{-150x^2}$	$y(0) = 1$	$0 \le x \le 20$	Russell[11]
5.	$y_1' = y_2$ $y_2' = -y_1$ Exact solution: $y_1(x) = \sin x$, $y_2(x) = \cos x$	$y_1(0) = 0$ $y_2(0) = 1$	$0 \le x \le 16\pi$	Shampine[13]
6.	$y_1' = 198y_1 + 199y_2$ $y_2' = -398y_1 - 399y_2$ Exact solution: $y_1(x) = e^{-x}$, $y_2(x) = -e^{-x}$	$y_1(0) = 1$ $y_2(0) = -1$	$0 \le x \le 20$	Burden[2]

Table 3.1: Results for Problem 1

Method	Tol	$N_{success}$	N_{reject}	N_{total}	$Step_r$	Max_{error}
GMBDF	10^{-2}	17	1	18	22.22%	1.85538e-02
BGMBDF		14	0	14		1.21930e-02
GMBDF	10^{-4}	33	4	37	29.73%	1.81471e-04
BGMBDF		26	0	26		1.24969e-04
GMBDF	10^{-6}	58	2	60	35.00%	1.26832e-06
BGMBDF		39	0	39		1.24997e-05

Table 3.2: Results for Problem 2

Method	Tol	$N_{success}$	N_{reject}	N_{total}	$Step_r$	Max_{error}
GMBDF	10^{-2}	22	3	25	12.00%	1.87456e-02
BGMBDF		22	0	22		5.09077e-02
GMBDF	10^{-4}	38	5	43	32.56%	2.45713e-04
BGMBDF		29	0	29		2.49875e-04
GMBDF	10^{-6}	68	5	73	38.36%	2.17301e-06
BGMBDF		45	0	45		2.49988e-05

Table 3.3: Results for Problem 3

Method	Tol	$N_{success}$	N_{reject}	N_{total}	$Step_r$	Max_{error}
GMBDF	10^{-2}	31	3	34	8.82%	3.08258e-02
BGMBDF		30	3	33		9.75807e-02
GMBDF	10^{-4}	56	4	60	16.67%	6.01461e-04
BGMBDF		47	3	50		8.96330e-05
GMBDF	10^{-6}	81	3	84	13.10%	2.30242e-06
BGMBDF		70	3	73		8.42803e-07

Table 3.4: Results for Problem 4

Method	Tol	$N_{success}$	N_{reject}	N_{total}	$Step_r$	Max_{error}
GMBDF		41	5	46	19.57%	4.43383e-03
BGMBDF	10^{-3}	33	4	37		1.22754e-03
GMBDF		58	9	67	25.37%	6.66952e-04
BGMBDF	10^{-4}	44	6	50		2.82904e-04
GMBDF		118	14	132	46.97%	7.14465e-07
BGMBDF	10^{-7}	68	2	70		1.91068e-07

Table 3.5: Results for Problem 5

Method	Tol	$N_{success}$	N_{reject}	N_{total}	$Step_r$	Max_{error}
GMBDF		76	4	80	22.50%	1.09651e+00
BGMBDF	10^{-2}	62	0	62		1.50633e-01
GMBDF		145	4	149	22.15%	6.66357e-03
BGMBDF	10^{-4}	116	0	116		7.87780e-04
GMBDF		246	9	255	28.24%	6.89557e-05
BGMBDF	10^{-6}	183	0	183		3.74168e-05

Table 3.6: Results for Problem 6

Method	Tol	$N_{success}$	N_{reject}	N_{total}	$Step_r$	Max_{error}
GMBDF		32	6	38	21.05%	4.46098e-02
BGMBDF	10^{-2}	27	3	30		1.93216e-02
GMBDF		38	5	43	18.60%	9.22114e-04
BGMBDF	10^{-4}	34	1	35		2.45713e-04
GMBDF		58	3	61	24.59%	2.19194e-05
BGMBDF	10^{-6}	45	1	46		1.24003e-05

4 Conclusions

The numerical results obtained using the block method described in this paper gives acceptable results. Comparing BGMBDF with GMBDF, we conclude that the former method is more efficient since the reductions in total step is almost one quarter for some tolerance chosen.

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