A-EBDF: an adaptive method for numerical solution of stiff systems of ODEs

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Abstract

In this paper a one parameter predictor–corrector method, which we call it A-EBDF, is introduced and analyzed. With a modification of A-BDF and EBDF methods we propose a multistep method whose region of absolute stability is larger than those of A-BDF and EBDF methods.

MSC: 65L05
Keywords: BDF, EBDF, Stability, Stiff ODEs

1. Introduction

Let us consider the stiff initial value problem

\[ y'(x) = f(x, y(x)), \quad y(x_0) = y_0 \]  

(1.1)

on the finite interval \( I = [x_0, x_N] \), where \( y : [x_0, x_N] \rightarrow \mathbb{R}^n \) and \( f : [x_0, x_N] \times \mathbb{R}^n \rightarrow \mathbb{R}^n \) is continuous. A-potentially good numerical method for the solution of stiff systems of ODEs must have good accuracy and some reasonably wide region of absolute stability [3]. A-stability requirement puts a severe limitation on the choice of a suitable methods for stiff problems. In the last 30 years or so, numerous works have been focusing on the development of more advanced and efficient methods for stiff problems. Most if these improvements in the class of linear multistep methods have been based on backward differentiation formula (BDF), because of its special properties.

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Among the first modification introduced by different authors was the extended backward differentiation formula (EBDF) introduced by Cash [1] in which one superfuture point technique was applied. This method is A-stable up to order 4 and A(α)-stable up to order 9. In the MEBDF (modified EBDF) [2] and MF-MEBDF (Matrix free MEBDF) [6], the authors tried to optimize the necessary computations of EBDF. With a blended application of implicit and explicit BDF, the so called A-BDF method was introduced by Fredebeul [4] which has one free parameter and is A(α)-stable up to order 7.

In this article a one parameter family of predictor–corrector schemes, which will be called A-EBDF, are obtained on the basis of a hybrid application of A-BDF and EBDF. Analyzing this new scheme it is shown that this method is A(α)-stable up to order 9 with a wider angle α, i.e., its region of stability is larger than those of A-BDF and EBDF. The accuracy here is superior to that of compared favorably with EBDFs. This article is organized as follows: Section 2 is devoted to the details of A-EBDF methods. In Section 3 the stability analysis is carried out and Section 4 will be devoted to some numerical examples of ODEs with different stiffness ratios and stability limitations.

2. Adaptive EBDF

In this section, with an interim mention of the algorithms EBDF and A-BDF and theirs properties, we derive our new algorithm A-EBDF.

2.1. EBDF scheme

This method that introduced in 1980 by Cash [1] is taking the following general form

$$
\sum_{j=0}^{k} \tilde{a}_j y_{n+j} = h \tilde{\alpha}_k f_{n+k} + h \tilde{\beta}_k f_{n+k+1},
$$

(2.1)

where \( \tilde{a}_k = 1 \) and the other coefficients are chosen so that (2.1) has order \( k+1 \). For the coefficients \( \tilde{\alpha}_k \) and \( \tilde{\beta}_k \) see [1].

Assuming that the solution values \( y_n, y_{n+1}, \ldots, y_{n+k-1} \) are available, the way in which (2.1) is used in practice is by following the below mentioned stages:

- **Stage 1.** Compute \( \tilde{y}_{n+k} \) as the solution of the \( k \)-step BDF

$$
y_{n+k} = h \tilde{\alpha}_k f_{n+k} - \sum_{j=0}^{k-1} a_j y_{n+j},
$$

(2.2)

- **Stage 2.** Compute \( \tilde{y}_{n+k+1} \) by solving the following algebraic equation

$$
y_{n+k+1} - h \tilde{\alpha}_k f_{n+k+1} = -a_{k-1} \tilde{y}_{n+k} - \sum_{j=0}^{k-2} a_j y_{n+j+1},
$$

(2.3)

- **Stage 3.** Evaluate

$$
\tilde{f}_{n+k+1} = f(x_{n+k+1}, \tilde{y}_{n+k+1})
$$
Table 1
The comparison of $A(\alpha)$-stability of A-EBDF with other mentioned methods

<table>
<thead>
<tr>
<th>$k$</th>
<th>BDF</th>
<th>A-BDF</th>
<th>EBDF</th>
<th>A-EBDF</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$p$</td>
<td>$\alpha$</td>
<td>$p$</td>
<td>$u_{\text{max}}$</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>90</td>
<td>1</td>
<td>90</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>90</td>
<td>2</td>
<td>90</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>88</td>
<td>3</td>
<td>90</td>
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<td>4</td>
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<td>73</td>
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<td>88</td>
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<td>5</td>
<td>5</td>
<td>51</td>
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<td>73</td>
</tr>
<tr>
<td>6</td>
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<td>18</td>
<td>6</td>
<td>51</td>
</tr>
<tr>
<td>7</td>
<td>7</td>
<td>–</td>
<td>7</td>
<td>18</td>
</tr>
<tr>
<td>8</td>
<td>8</td>
<td>–</td>
<td>8</td>
<td>–</td>
</tr>
</tbody>
</table>

- Stage 4. Compute $y_{n+k}$ as the solution of

$$y_{n+k} - h\hat{\beta}_k f_{n+k} = - \sum_{j=0}^{k-1} \hat{\alpha}_j y_{n+j} + h\hat{\beta}_k f_{n+k+1}$$

for the coefficients $\beta_k$ and $\alpha_j$ see [8].

**Lemma 2.1.** Given that
(i) formula (2.2) is of order $k$,
(ii) formula (2.1) is of order $k+1$,
(iii) the implicit algebraic equations defining $\bar{y}_{n+k}$ and $\bar{y}_{n+k+1}$ are solved exactly, then formula (2.4) has
order $k+1$.

For proof see [5].

As we know the EBDF scheme is $A(\alpha)$-stable for $k = 1, 2, \ldots, 8$ and in Table 1 we list the angles of $\alpha$.

### 2.2. A-BDF

This method, that is introduced by Fredebeul, has a large stability region, compared to BDF. It is a blended method of implicit and explicit BDF that is defined as follows:

$$\text{BDF}^{(i)}_{\text{I}} : \sum_{j=0}^{k} \delta_j y_{n+j} = h\hat{\beta}_k f_{n+k-1}$$

$$\text{BDF}^{(ii)}_{\text{I}} : \sum_{j=0}^{k} \alpha_j y_{n+j} = h\beta_k f_{n+k}$$

where $\alpha_0 = \bar{\alpha}_k = 1$ and the other coefficients are chosen so that above schemes have order $k$. 
Then the corresponding adaptive BDF of degree \( k \), or A-BDF \( k \) for short, is given by

\[
\text{BDF}_k^{(i)} - t \text{BDF}_k^{(i)} = 0
\]

or

\[
\sum_{j=0}^{k} (a_j - t̄a_j)y_{n+j} = h\hat{\theta}_k f_{n+k} - h\hat{\theta}_k f_{n+k-1}
\]  \( (2.7) \)

- for all \( t \in \mathbb{R} - \{1\} \) the method is of order \( k \),
- for some value of \( t \), the method is zero-stable for \( k = 1, 2, \ldots, 7 \)
- the A-BDF \( k \) is \( A(\alpha) \)-stable for \( k = 1, 2, \ldots, 7 \) and the angles of \( \alpha \) are listed in Table 1. For details see [4].

2.3. A-EBDF

Now we define an adaptive \( k \)-step formula as follows.

In the EBDF algorithm we use A-BDF scheme for predictors in stages 1 and 2 and correct \( y_{n+k} \) by the same formula (2.1).

So by assuming that the solution values \( y_n, y_{n+1}, \ldots, y_{n+k-1} \) are available, to compute \( y_{n+k} \) we carry out the following stages:

- **Stage 1.** Compute \( \tilde{y}_{n+k} \) as the solution of the \( k \)-step A-BDF

\[
\sum_{j=0}^{k} (a_j - t\tilde{a}_j)y_{n+j} = h\hat{\theta}_k f_{n+k} - h\hat{\theta}_k f_{n+k-1}
\]  \( (2.8) \)

- **Stage 2.** Compute \( \tilde{y}_{n+k+1} \) as the solution of

\[
\sum_{j=0}^{k} (a_j - t\tilde{a}_j)y_{n+j+1} = h\hat{\theta}_k f_{n+k+1} - h\hat{\theta}_k f_{n+k}
\]  \( (2.9) \)

- **Stage 3.** Evaluate

\[
\tilde{f}_{n+k+1} = f(x_{n+k+1}, \tilde{y}_{n+k+1})
\]

- **Stage 4.** Correct \( y_{n+k} \) as the solution of

\[
y_{n+k} - h\hat{\theta}_k f_{n+k} = \sum_{j=0}^{k-1} \tilde{a}_j y_{n+j} + h\hat{\theta}_k f_{n+k+1}
\]  \( (2.10) \)

We note that in implementing stages 1, 2 and 4 to integrate a nonlinear initial value problem, it is necessary to solve a system of nonlinear algebraic equation for each of the required solutions \( y_{n+k}, \tilde{y}_{n+k+1} \) and \( y_{n+k} \).

In each case, these algebraic equations are solved using a modified form of Newton iteration *iterated to convergence.*
By an analogous result of Lemma 2.1, for all values of \( t \in \mathbb{R} - \{1\} \) this scheme is of order \( k + 1 \). For \( t = 0 \), one obtains EBDF.

Of course the analogical one parameter methods is introduced that in those the parameter is appeared only in right hand of relation. See e.g. [7].

3. Stability analysis

We now examine the stability behavior of our approach and determine the restrictions which we need to impose on the free parameter to obtain highly stable methods. If we apply (2.8) to the test problem \( y' = \lambda y \), we get

\[
y_{n+k} = - \sum_{j=0}^{k-1} \frac{\alpha_j - \tilde{\alpha}_j}{1 - t - h\hat{\beta}_k} y_{n+j} - \frac{\tilde{\alpha}_0 \hat{\beta}_k h}{1 - t - h\hat{\beta}_k} y_{n+k-1}, \tag{3.1}
\]

where \( \hat{h} = \lambda h \), and from (2.9) we obtain

\[
y_{n+k+1} = - \sum_{j=0}^{k-2} \frac{\alpha_j - \tilde{\alpha}_j}{1 - t - h\hat{\beta}_k} y_{n+k+1} - \frac{\alpha_{k-1} - \tilde{\alpha}_{k-1} + \hat{\beta}_k}{1 - t - h\hat{\beta}_k} y_{n+k}, \tag{3.2}
\]

substituting (3.1) into (3.2) and collecting the terms, we obtain an expression of the form

\[
\tilde{y}_{n+k+1} = \sum_{j=0}^{k-1} \gamma_j y_{n+j}, \tag{3.3}
\]

where

\[
\gamma_0 = \frac{(\alpha_0 - \tilde{\alpha}_0)(\alpha_{k-1} - \tilde{\alpha}_{k-1} + \hat{\beta}_k)}{(1 - t - h\hat{\beta}_k)^2},
\]

\[
\gamma_j = \frac{-(\alpha_{j-1} - \tilde{\alpha}_{j-1})(1 - t - h\hat{\beta}_k) + (\alpha_j - \tilde{\alpha}_j)(\alpha_{k-1} - \tilde{\alpha}_{k-1} + \hat{\beta}_k)}{(1 - t - h\hat{\beta}_k)^2}, \quad j = 1, 2, \ldots, k - 2,
\]

\[
\gamma_{k-1} = \frac{-(\alpha_{k-2} - \tilde{\alpha}_{k-2})(1 - t - h\hat{\beta}_k) + (\alpha_{k-1} - \tilde{\alpha}_{k-1} + \hat{\beta}_k)^2}{(1 - t - h\hat{\beta}_k)^2}.
\]

If we apply (2.10) to the same scalar test equation we get

\[
(1 - \hat{h}\hat{\beta}_k) y_{n+k} = - \sum_{j=0}^{k-1} \tilde{\alpha}_j y_{n+j} + \hat{\beta}_k y_{n+k+1}. \tag{3.4}
\]

Substituting (3.3) into (3.4), we have

\[
\sum_{j=0}^{k} C_j(\hat{h}) y_{n+j} = 0,
\]
The values of $t_{opt}$ for maximum angle $\alpha$ in A-EBDF

<table>
<thead>
<tr>
<th>$k$</th>
<th>$t_{opt}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$[-5.65, 0.15]$</td>
</tr>
<tr>
<td>2</td>
<td>$[-0.781, 0.745]$</td>
</tr>
<tr>
<td>3</td>
<td>$[-0.524, 1)$</td>
</tr>
<tr>
<td>4</td>
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</tr>
<tr>
<td>5</td>
<td>$-0.33$</td>
</tr>
<tr>
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<td>$-0.28$</td>
</tr>
<tr>
<td>7</td>
<td>$-0.25$</td>
</tr>
<tr>
<td>8</td>
<td>$-0.14$</td>
</tr>
</tbody>
</table>

where

$C_k = 1 - \tilde{h}\hat{\beta}_k,$

$C_j = \tilde{\alpha}_j - \tilde{h}\hat{\beta}_{k+1}y_j', j = 0, 1, \ldots, k - 1.$

Therefore, corresponding characteristic equation of the $k$th order difference equation of the A-EBDF is

$$\pi(\xi, \tilde{h}) = \sum_{j=0}^{k} C_j \xi^j = 0. \tag{3.5}$$

If in (3.5) we put $\tilde{h} = \lambda h = 0$, then by a theorem of Schur [8], we conclude that A-EBDF for $t \in \mathbb{R} - \{1\}$, satisfies the root condition.

To obtain the region of absolute stability we use the boundary locus method [9]. By collecting coefficients of powers of $\tilde{h}$ in (3.5), we have

$$A\tilde{h}^3 + B\tilde{h}^2 + C\tilde{h} + D = 0, \tag{3.6}$$

where $A, B, C, D$ are functions of $\xi$. Inserting $\xi = e^{i\theta}$, Eq. (3.6) gives us three roots $\tilde{h}_i(\theta)$, $i = 1, 2, 3$, which describe the stability domain.

The A-EBDF is $A$-stable for $p \leq 4$ and is $A(\alpha)$-stable for orders up to 9 with a wider angle $\alpha$, compared with BDF, A-BDF and EBDF. This comparison can be seen in Table 1. For example, for $k = 8$ the EBDF is $A(19.96)$-stable, while A-EBDF is $A(30.50)$-stable, so is capable of producing stable numerical solution for a larger class of stiff ODEs. The values of $t_{opt}$ and its corresponding maximum value of $\alpha$ for $k = 1, 2, \ldots, 8$ are listed in Table 2.

4. Numerical results

In this section we present some numerical results to compare the performance of A-EBDF with that of EBDF and BDF. We need to emphasize that we shall not compare accuracy of new method with that of EBDF.

Example 4.1. The following problem has been considered by Cash [1] to compare EBDF and BDF schemes. It is a reactor kinetics problem suggested by Liniger and Willoughby [9].

$$y_1' = (0.01 + y_1 + y_2)(y_1^0 + 1001y_1 + 1001), \quad y_2' = (0.01 + y_1 + y_2)(1 + y_2^0)$$

with initial value $y(0) = (0, 0)^T$. 

Table 2
The values of $t_{opt}$ for maximum angle $\alpha$ in A-EBDF

<table>
<thead>
<tr>
<th>$k$</th>
<th>$t_{opt}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
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</tr>
</tbody>
</table>
In Table 3 we list the error of the computed solution obtained by the A-EBDF and compare it with those given by Cash for EBDF and BDF. To evaluate the approximation values of the solution at a given \( x \), the step-length \( h = x/10 \) is used and in A-EBDF with \( k = 6 \), we put \( t = -0.2 \).

**Example 4.2.** Consider another stiff system:
\[
\begin{align*}
y'_1 &= -y_1 - 15y_2 + 15e^{-x}, \\
y'_2 &= 15y_1 - y_2 - 15e^{-x}
\end{align*}
\]
with initial value \( y(0) = (1, 1)^T \).

Its exact solution is
\[
y_1(x) = y_2(x) = e^{-x}.
\]
This system has eigenvalues of large modulus lying close to the imaginary axis \(-1 \pm 15i\). It can be seen that the 4-step BDF becomes unstable whereas the 3-step EBDF and 6-step A-EBDF (with \( t = -0.2 \)) remains stable. We tabulate the error results in Table 4.

**Example 4.3.** The following stiff initial value problem arose from a chemistry problem
\[
\begin{align*}
y'_1 &= -0.013y_2 - 1000y_1y_2 - 2500y_2y_3, \\
y'_2 &= -0.013y_2 - 1000y_1y_2, \\
y'_3 &= -2500y_2y_3
\end{align*}
\]
with initial value \( y(0) = (0, 1, 1)^T \).

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\end{align*}
\]
with initial value \( y(0) = (0, 1, 1)^T \).
Table 5
Results for integration of example 4.3

<table>
<thead>
<tr>
<th>x</th>
<th>$y_1$</th>
<th>Exact solution</th>
<th>Error in A-EBDF</th>
<th>Error in EBDF</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>$y_1$</td>
<td>$-0.361693169289E-5$</td>
<td>0.57E-09</td>
<td>0.46E-10</td>
</tr>
<tr>
<td></td>
<td>$y_2$</td>
<td>0.9815029948230</td>
<td>0.22E-06</td>
<td>0.91E-07</td>
</tr>
<tr>
<td></td>
<td>$y_3$</td>
<td>1.01849398244</td>
<td>0.22E-06</td>
<td>0.92E-07</td>
</tr>
</tbody>
</table>

Table 6
Results for integration of example 4.4

<table>
<thead>
<tr>
<th>x</th>
<th>$y_1$</th>
<th>Exact solution</th>
<th>Error in A-EBDF</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>$y_1$</td>
<td>0.303265331217737E-0</td>
<td>0.38E-07</td>
</tr>
<tr>
<td></td>
<td>$y_2$</td>
<td>0.303265330376617E-0</td>
<td>0.39E-07</td>
</tr>
<tr>
<td></td>
<td>$y_1$</td>
<td>$-0.30326532936316E-0$</td>
<td>0.38E-07</td>
</tr>
<tr>
<td>5.0</td>
<td>$y_1$</td>
<td>0.410424993119494E-1</td>
<td>0.14E-08</td>
</tr>
<tr>
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<td>0.410424993119494E-1</td>
<td>0.14E-08</td>
</tr>
<tr>
<td></td>
<td>$y_1$</td>
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</tr>
<tr>
<td>10.0</td>
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<td>0.22E-09</td>
</tr>
<tr>
<td></td>
<td>$y_2$</td>
<td>0.336897349954273E-2</td>
<td>0.22E-09</td>
</tr>
<tr>
<td></td>
<td>$y_1$</td>
<td>$-0.336897349954273E-2$</td>
<td>0.22E-09</td>
</tr>
</tbody>
</table>

We solve this problem at $x = 2$ and tabulate the results in Table 5.

**Example 4.4.** Consider the system of differential equations:

\[
y'_1 = -20y_1 - 0.25y_2 - 19.75y_3, \quad y'_2 = 20y_1 - 20.25y_2 + 0.25y_3, \quad y'_3 = 20y_1 - 19.75y_2 - 0.25y_3
\]

with initial value $y(0) = (1, 0, -1)^T$.

The theoretical solution is

\[
y_1 = \frac{1}{2}(e^{-0.5x} + e^{-20x}(\cos(20x) + \sin(20x))), \quad y_2 = \frac{1}{2}(e^{-0.5x} - e^{-20x}(\cos(20x) - \sin(20x))),
\]

\[
y_3 = -\frac{1}{2}(e^{-0.5x} + e^{-20x}(\cos(20x) - \sin(20x))).
\]

The system is integrated by A-EBDF and the results are tabulated in Table 6 at different values of $x$.

References


