数理解析研究所講究録
第 676 巻 1988 年 126-136

On the Existence Theorems of BDF and Adams type Second Derivative BDF with Nonnegative Coefficients

K.Ozawa (Sendai National College of Technology)
小沢　一文（仙台電波高専）

1. Introduction

The backward differentiation formulas (BDF)

$$\alpha_k\, y_{n+k} + \alpha_{k-1}\, y_{n+k-1} + \cdots + \alpha_0\, y_n = h\, \beta_k\, f_{n+k} \tag{1.1}$$

are the most widely used methods for the solution of stiff differential equations. These formulas were proved to be stable for $k<7$ by Cryer (1972) and Hairer & Wanner (1983). Enright (1974) extended the BDF to the Adams type methods which evaluate the second derivative of the solution. The Enright's formulas are of the form

$$y_{n+k} - y_{n+k-1} = h(\beta_k f_{n+k} + \beta_{k-1} f_{n+k-1} + \cdots + \beta_0 f_n) + h^2 \delta_k f'_{\ n+k} \tag{1.2}$$

and were proved to be stiff-stable for $k<8$ (see Enright (1974) and Jeltsch (1977)). Although the formulas (1.1) and (1.2) are highly stable, the coefficients of these formulas have mixed signs except for $k=1$, implying that these methods are vulnerable to the cancellation of significant figures.

In this article, we shall be concerned with the BDF and with the Adams type second derivative BDF (SBDF) having nonnegative coefficients. Ozawa (1988) proposed some linear multistep methods with nonnegative coefficients, and proved that the methods are more accurate than Adams-Moulton methods.

2. Preliminary

Let consider the linear multistep method,

$$\sum_{i=0}^{k} \alpha_i\, y_{n+i} = \sum_{i=0}^{k} \sum_{j=1}^{l} h^j\, \beta_{ij}\, f_{n+i}^{(j-1)}\,, \quad n=0,1,\cdots,N-k, \tag{2.1}$$

for solving the initial value problem

$$y' = f(x,y), \quad y(x_0) = \eta, \quad x_0 \le x \le x_N. \tag{2.2}$$

where

$$f_i^{(j)} = f^{(j)}(x_i,y_i),$$

$$f^{(j)}(x,y) = \frac{d}{dx} f^{(j-1)}(x), \quad j=1,2,\cdots,l-1,$$

$$x_i = x_0 + ih, \quad i=0,1,\cdots,N.$$

We say that the methods (2.1) are (k,l)-methods if

$$\alpha_k > 0, \quad \sum_{i=0}^{k} |\beta_{il}| > 0. \tag{2.3}$$

It is convenient to associate with the (k,l)-methods the following polynomials:

$$\rho(\zeta) = \sum_{i=0}^{k} \alpha_i \zeta^i, \quad \sigma_j(\zeta) = \sum_{i=0}^{k} \beta_{ij} \zeta^i, \quad j=1,2,\cdots,l. \tag{2.4}$$

Moreover, we associate with the (k,l)-methods the difference operator

$$L[\, y(x); h] = (\rho(E) - \sum_{j=1}^{l} \sigma_j(E)\, h^j D^j\,)\, y(x), \tag{2.5}$$

where D is the differential operator and E is the shift operator, i.e.,

$$Dy(x) = \frac{d}{dx} y(x), \quad Ey(x) = y(x+h).$$

The order of the methods (2.1) are said to be p if for all $y \in C^{(p+1)}[x_0,x_N]$

$$L[\, y(x); h] = C_{p+1}\, h^{p+1} y^{(p+1)}(x) + O(h^{p+2}), \quad h \to 0. \tag{2.6}$$

where C_{p+1} is a nonzero constant independent of h. Let $y(x)=e^x$ and $\zeta=e^h$, then

$$L[\, e^x; h] = [\, \rho(\zeta) - \sum_{j=1}^{l} \sigma_j(\zeta)\, h^j\,] e^x$$

$$= C_{p+1}\, h^{p+1}\, e^x + O(h^{p+2}), \quad h \to 0. \tag{2.7}$$

Using the variable $t = 1 - \zeta^{-1}$, we have from (2.7),

$$-\frac{R(t)}{\log(1-t)} - \sum_{j=1}^{l} (-1)^{j-1} S_j(t) [\log(1-t)]^{j-1} = C_{p+1} t^p + O(t^{p+1}), \quad t \to 0, \tag{2.8}$$

where $R(t)$, $S_j(t)$ are the polynomials of degree$\leq k$ and are given by

$$R(t) = \zeta^{-k}\rho(\zeta), \quad S_j(t) = \zeta^{-k}\sigma_j(\zeta), \quad j=1,2,\cdots,l. \tag{2.9}$$

In the succeeding sections we will use the eq. (2.8) to determine the coefficients α_j, β_{ij} of the methods (2.1).

3. BDF with nonnegative coefficients

For the formula of the type (1.1), $l=1$ and

$$\sigma_1(\zeta) = \zeta^k, \quad S_1(t) = 1, \tag{3.1}$$

and consequently eq. (2.8) reduces to

$$-\frac{R(t)}{\log(1-t)} - 1 = C_{p+1}\,t^p + O(t^{p+1}), \quad t\to 0. \tag{3.2}$$

Since $R(t)$ is a polynomial of degree$\leq k$, the order attainable with the method is k. The k-step BDF derived by Gear (1971) has the maximal order k, but the coefficients of the formula for $k>1$ does not satisfy the condition of nonnegativeness, i.e.,

$$\alpha_k>0, \quad -\alpha_j\geq 0, \quad j=0,1,\cdots,k-1. \tag{3.3}$$

Now, we find the methods of the type (1.1) with the condition (3.3), by decreasing the order by one against the maximal order. Putting $p=k-1$, we have from (3.2)

$$R(t) = t + \frac{t^2}{2} + \cdots + \frac{t^{k-1}}{k-1} + at^k, \tag{3.4}$$

where a is a free parameter taken to be consistent with the condition (3.3). The coefficients α's obtained from (3.4) are

$$\alpha_{k-i} = (-1)^i \binom{k}{i} \left[a - \left(\frac{1}{k} - \frac{1}{i}\right) \right], \quad i=1,2,\cdots,k, \tag{3.5}$$

$$\alpha_k = \sum_{j=1}^{k-1}\frac{1}{j} + a. \tag{3.6}$$

Next we derive the interval of a from eqs. (3.5) and (3.6) in which the coefficients α's satisfy the condition (3.3). Taking into account

$$-\sum_{j=1}^{k-1}\frac{1}{j} < \frac{1}{k} - \frac{1}{i}, \quad i>0,$$

we can easily see that such interval is given by

$$L \equiv \max_{\substack{i=odd\\0<i\leq k}} \left(\frac{1}{k} - \frac{1}{i} \right) \leq a \leq \min_{\substack{i=even\\0<i\leq k}} \left(\frac{1}{k} - \frac{1}{i} \right) \equiv U. \tag{3.7}$$

The inequality appeared in (3.7) is valid only for even k, since for odd k we have L=0, U<0. On the other hand, if k is an even number>2 then we have another contradiction

$$U = \frac{1}{k} - \frac{1}{2} < \frac{1}{k} - \frac{1}{k-1} = L. \tag{3.8}$$

This result suggests that the inequality (3.7) is valid only for k=2. In fact, if k=2, then L=−1/2, U=0. Thus we have proved the following Theorem:
Theorem 1

The BDF (1.1) satisfy the nonnegative condition (3.3) only for k=2, *and the formulas are*

$$(1+a)y_{n+2} - (1+2a)y_{n+1} + ay_n = hf_{n+2}, \tag{3.10}$$

$$-\frac{1}{2} \leq a \leq 0,$$

$$C_2 = a - \frac{1}{2}.$$

In the family (3.10) *the method corresponding to a=0 is the well-known backward Euler formula, which minimizes the absolute value of the error constant* C_2.

Next we show that the family (3.10) is A-stable. We can see that the boundary locus of the absolute stability region of the family is given by

$$Z(\theta) = (1+a) - (1+2a)e^{-i\theta} + ae^{-2i\theta}, \tag{3.11}$$

and it's real part is given by

$$\mathrm{Re}[Z(\theta)] = (2ax-1)\,(x-1), \tag{3.12}$$

where

$$x = \cos\theta.$$

The relation (3.12) shows that if $-\frac{1}{2} \leq a \leq 0$, then $\mathrm{Re}[Z(\theta)]>0$ exept for $|x|=1$. Consequently $Z(\theta)$ is a closed locus on the right half-plane, i.e., the family (3.10) is A-stable.

We have now obtained a class of 2-step BDF of order 1 with the nonnegative condition (3.3), by decreasing the order by one against the maximal one. It may be expected that the BDF with nonnegative coefficients have order$\geq$2, if we would decrease the order by two or more against the maximal one. However, the next Theorem shows that it is quite impossible to have order$\geq$2 for the BDF with nonnegative coefficients.

Theorem 2

Let the coefficients of the BDF satisfy the condition (3.3), then the BDF must have order<2.

[Proof] For the BDF, the power series expansion of the operator (2.5) is as follows (see Lambert (1974)):

$$L[\, y(x);\, h] = \sum_{j=0}^{k} \alpha_j\, y(x+jh) - h\, f(x,y(x)) \tag{3.13}$$

$$= C_0 y(x) + C_1 y^{(1)}(x)\, h + C_2 y^{(2)}(x)\, h^2 + \cdots,$$

where

$$C_0 = \alpha_0 + \alpha_1 + \cdots + \alpha_k, \tag{3.14}$$

$$C_1 = \alpha_1 + 2\alpha_2 + \cdots + k\alpha_k - 1,$$

$$C_q = \frac{1}{q!}\sum_{j=1}^{k} j^q\, \alpha_j - \frac{1}{(q-1)!}\, k^{q-1}, \quad q\geq 2.$$

Using this relation, we can find

$$C_2 = -\frac{k^2}{2} C_0 + kC_1 + \frac{1}{2}\sum_{j=1}^{k} j^2\, \alpha_{k-j}. \tag{3.15}$$

In order that the BDF have order$\geq$2, it is necessary that

$$C_0 = C_1 = C_2 = 0. \tag{3.16}$$

But, if we set $C_0 = C_1 = C_2 = 0$ in (3.15), then we have

$$\alpha_j = 0, \quad j=0,1,\cdots,k. \tag{3.17}$$

Cleary this contradicts the condition (3.3). Q.E.D.

4. Adams type SBDF with nonnegative coefficients

In this section, we find the Adams type SBDF with nonnegative coefficients using the same way as in the preceding section. For the Adams type SBDF (1.2), l=2 and

$$\begin{aligned}\rho(\zeta) &= \zeta^{k} - \zeta^{k-1}, \qquad (4.1)\\ \sigma_1(\zeta) &= \beta_{k1}\zeta^{k} + \beta_{k-11}\zeta^{k-1} + \cdots + \beta_{01},\\ \sigma_2(\zeta) &= \delta_k\zeta^{k}.\end{aligned}$$

For this case, eq. (2.8) reduces to

$$-\frac{R(t)}{\log(1-t)} - S_1(t) + S_2(t)\log(1-t) = C_{p+1}t^{p} + O(t^{p+1}), \quad t\to 0, \qquad (4.2)$$

where

$$R(t) = t, \quad S_1(t) = \zeta^{-k}\sigma_1(\zeta), \quad S_2(t) = \delta_k.$$

In order to simplify the notation we omit the second index of β's and put $\delta_k=a$. The function $-t/\log(1-t)$ has the expansion (see Henrici (1962)),

$$-\frac{t}{\log(1-t)} = \gamma_0^* + \gamma_1^*\, t + \gamma_2^*\, t^2 + \cdots, \quad t\to 0, \qquad (4.3)$$

$$\gamma_j^* = (-1)^j \int_{-1}^{0} \binom{-s}{j}\, ds, \quad j=0,1,2,\cdots, \qquad (4.4)$$

and

$$\log(1-t) = -\left(t + \frac{t^2}{2} + \frac{t^3}{3} + \cdots\right), \quad t\to 0. \qquad (4.5)$$

Therefore, if we set in (4.2)

$$S_1(t) = \gamma_0^* + (\gamma_1^* - a)\, t + \cdots + \left(\gamma_k^* - \frac{a}{k}\right) t^k, \qquad (4.6)$$

then the method (1.2) has order $p=k+1$ and, moreover, if we set $a=(k+1)\gamma_{k+1}^*$ then the order is increased up to $p=k+2$. The k-step Enright's method has this maximal order $k+2$, but the coefficients have mixed signs for $k>1$.

Here we have to determine the coefficients β's so as to satisfy the nonnegative condition

$$\beta_j \geq 0, \quad j=0,1,\cdots,k, \tag{4.7}$$

by decreasing the order by one against the maximal one. From (4.6), it can be seen that the coefficients β's are given by

$$\beta_{k-i} = (-1)^i \left[\sum_{j=i}^{k} \binom{j}{i} \gamma_j^* - \binom{k}{i} i^{-1} a \right], \quad i=1,2,\cdots,k, \tag{4.8}$$

$$\beta_k = \sum_{j=0}^{k} \gamma_j^* - a \sum_{j=1}^{k} \frac{1}{j}, \tag{4.9}$$

where the formula

$$\binom{r}{r} + \binom{r+1}{r} + \cdots + \binom{s}{r} = \binom{s+1}{r+1}, \quad s>r \tag{4.10}$$

is used. In order that the coefficients of the method to be nonnegative, the parameter a should be contained in the interval

$$L \equiv \max_{\substack{i=odd \\ 0\leq i\leq k}} T_i^{(k)} \leq a \leq \min_{\substack{i=even \\ 0\leq i\leq k}} T_i^{(k)} \equiv U, \tag{4.11}$$

where

$$T_0^{(k)} = \left(\sum_{j=1}^{k} \frac{1}{j}\right)^{-1} \sum_{j=0}^{k} \gamma_j^*, \tag{4.12a}$$

$$T_i^{(k)} = \binom{k}{i}^{-1} i \sum_{j=i}^{k} \binom{j}{i} \gamma_j^*, \quad i=1,2,\cdots,k. \tag{4.12b}$$

The quantity $T_i^{(k)}$ satisfies the following Lemma:

Lemma

(a) $T_0^{(k)} > 0$,

(b) $T_i^{(k)} < 0$, for $i > 0$,

(c) $T_{i+1}^{(k)} - T_i^{(k)} > 0$, for $i > 0$.

[Proof] The constant γ_j^* has the following properties (see Henrici (1962)):

$$\gamma_j^* < 0, \quad j=1,2,\cdots, \tag{4.13}$$

$$\sum_{j=0}^{m} \gamma_j^* = (-1)^m \int_0^1 \binom{-s}{m} ds > 0. \tag{4.14}$$

From these properties the first two assertions are clear. For the proof of (c), we first show that $T_i^{(k)}$ is given by

$$T_i^{(k)} = \frac{i}{k!} \int_{-1}^{0} \prod_{\substack{l=0 \\ l\neq i}}^{k} (s+l)\, ds, \qquad i=1,2,\cdots,k. \tag{4.15}$$

To prove this we substitute (4.4) into (4.12b), then we have

$$\begin{aligned}
T_i^{(k)} &= \binom{k}{i}^{-1} i \sum_{j=i}^{k} \int_{-1}^{0} (-1)^j \binom{-s}{j} \binom{j}{i}\, ds \\
&= \binom{k}{i}^{-1} i \int_{-1}^{0} \sum_{j=i}^{k} \binom{s+j-1}{j} \binom{j}{i}\, ds \\
&= \frac{(k-i)!\, i}{k!} \int_{-1}^{0} \prod_{l=0}^{i-1} (s+l) \sum_{j=i}^{k} \binom{s+j-1}{s+i-1}\, ds \\
&= \frac{(k-i)!\, i}{k!} \int_{-1}^{0} \prod_{l=0}^{i-1} (s+l) \binom{s+k}{s+i}\, ds,
\end{aligned} \tag{4.16}$$

where the formula (4.10) is used. Thus (4.15) is obtained. Using (4.15), we have

$$T_{i+1}^{(k)} - T_i^{(k)} = \frac{1}{k!} \int_{-1}^{0} s^2 \prod_{\substack{l=1 \\ l\neq i,i+1}}^{k} (s+l)\, ds, \qquad i>0. \tag{4.17}$$

Since in this expression the integrand is positive on (-1,0), the assertion is followed. Q.E.D.

From this Lemma, the following results are derived:

$$L = \max_{\substack{i=odd \\ 0\leq i\leq k}} T_i^{(k)} = \begin{cases} T_k^{(k)} & ;\ k=odd, \\ T_{k-1}^{(k)} & ;\ k=even, \end{cases} \tag{4.18}$$

$$U = \min_{\substack{i=even \\ 0\leq i\leq k}} T_i^{(k)} = \begin{cases} T_2^{(k)} & ;\ k\geq 2, \\ T_0^{(k)} & ;\ k=1. \end{cases} \tag{4.19}$$

Using this result, for $k\geq 3$, we have a contradiction

$$U = T_2^{(k)} < T_3^{(k)} \leq L, \tag{4.20}$$

while for $k<3$, we have

$$k = 1: \qquad L = T_1^{(1)} < 0 < T_0^{(1)} = U, \tag{4.21}$$

$$k = 2: \qquad L = T_1^{(2)} < T_2^{(2)} = U.$$

Thus we have proved the next Theorem:

Theorem 3

The k-step Adams type SBDF of order k+1 have nonnegative coefficients only for k=1,2, and the families of the formulas are as follows:

(A1) 1-step method

$$y_{n+1} - y_n = h\left[(\frac{1}{2}-a)\, f_{n+1} + (\frac{1}{2}+a)\, f_n\right] + h^2\, a\, f'_{n+1}, \tag{4.22}$$

$$-\frac{1}{2} \le a \le \frac{1}{2},$$

$$C_3 = -\frac{1}{12} - \frac{a}{2}.$$

(A2) 2-step method

$$y_{n+2} - y_{n+1} = h\left[(\frac{5}{12}-\frac{3}{2}a)\, f_{n+2} + (\frac{2}{3}+2a)\, f_{n+1} - (\frac{1}{12}+\frac{a}{2})\, f_n\right]$$

$$+ h^2 a\, f'_{n+2}, \tag{4.23}$$

$$-\frac{1}{3} \le a \le -\frac{1}{6},$$

$$C_4 = -\frac{1}{24} - \frac{a}{3}.$$

In each of the formulas (4.22) and (4.23) if we set the parameter a so as to make the error constant 0, then the method becomes the Enright's method; *1-step Enright's method is included in the family A1 while 2-step Enright's method is not included in the family A2.*

We have obtained the Adams type SBDF of orders 2 and 3 with nonnegative coefficients. On the other hand, formulas of higher-order are more desirable than those of middle or low order, if higher accuracy is required. However, the next Theorem shows that it is impossible to have order$\geq$4 for the Adams type SBDF with nonnegative coefficients, even if we would decrease the order by two or more against the maximal one.

Theorem 4

The Adams type SBDF (1.2) with nonnegative coefficients must have order<4.

[Proof] As before we first give the power series expansion of the operator (2.5) for the formula (1.2). The power series is

$$L[\, y(x); h] = C_0 y(x) + C_1 y^{(1)}(x)\, h + C_2 y^{(2)}(x)\, h^2 + \cdots, \tag{4.24}$$

where

$$C_0 = 0, \tag{4.25}$$

$$C_1 = 1 - \sum_{j=0}^{k} \beta_j,$$

$$C_q = \frac{k^q - (k-1)^q}{q!} - \frac{1}{(q-1)!} \sum_{j=0}^{k} j^{q-1} \beta_j - \frac{a}{(q-2)!} k^{q-2}, \quad q \geq 2.$$

Consider the series $\{g_q\}$ defined by

$$g_q = \sum_{j=0}^{k} j^{q-1} \beta_{k-j}, \qquad q \geq 1, \tag{4.26}$$

where we define $0^0=1$. If $\beta_j \geq 0$, the series $\{g_q\}$ have the monotonicity

$$g_q \leq g_{q+1}, \quad q \geq 2. \tag{4.27}$$

After tedious calculations, we find the relation

$$g_1 = 1 - C_1,$$

$$g_2 = \frac{1}{2} + a - kC_1 + C_2, \tag{4.28}$$

$$g_q = \frac{1}{q} + \sum_{l=1}^{q} (-1)^l \, (l-1)! \, \binom{q-1}{l-1} \, k^{q-1} C_l, \quad q \geq 3.$$

In order that the method has order≥ 4 then it is necessary that

$$C_1 = C_2 = C_3 = C_4 = 0. \tag{4.29}$$

Substituting this into (4.28), we have

$$g_1 = 1, \;\; g_2 = \frac{1}{2} + a, \;\; g_3 = \frac{1}{3}, \;\; g_4 = \frac{1}{4}. \tag{4.30}$$

However, this result contradicts the monotonicity (4.27). Thus the assertion is proved. Q.E.D.

5. Conclusion

We have derived the following formulas with nonnegative coefficients:

(i) BDF of order 1,

(ii)Adams type SBDF (second derivative BDF) of orders 2 and 3.

Moreover, we have shown that the attainable order with these methods are 1 and 3, respectively.

References

[1]Cryer, C. W.(1972), *On the Instability of High Order Backward-Difference Multistep Methods,* BIT **12,** pp.17-25.

[2]Enright, W. H.(1974), *Second Derivative Multistep Methods for Stiff Ordinary Differential Equations,* SIAM J. Numer. Anal. **11,** pp.321-331.

[3]Gear, C. W.(1971), *Numerical Initial Value Problems in Ordinary Differential Equations,* Prentice-Hall, Englewood Cliffs, N.J.

[4]Hairer, E. and Wanner, G.(1983), *On the Instability of the BDF formulas,* SIAM J. Numer. Anal. **20,** pp.1206-1209.

[5]Henrici, P.(1962), *Discrete Variable Methods in Ordinary Differential Equations,* John Wiley & Sons Inc., New York.

[6]Jeltsch, R.(1977), *Multistep Methods Using Higher Derivatives and Damping at Infinity,* Math. of Comp. **31,** pp.124-138.

[7]Lambert, J. D.(1973), *Computational Methods in Ordinary Differential Equations,* John Wiley & Sons, New York.

[8]Ozawa, K.(1988), *On the Existence Theorems of Some Linear Multistep Methods with Nonnegative Coefficients* (in Japanese), RIMS Kokyuroku **643,** pp.94-116.