Implicit Linear Multistep Methods with Nonnegative Coefficients for Solving Initial Value Problems

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Consider the linear multistep methods (LM methods)

$$y_{n+k}+\alpha_{k-1}y_{n+k-1}+\ldots+\alpha_0 y_n=h(\beta_k f_{n+k}+\ldots+\beta_0 f_n)$$

for solving initial value problems of ordinary differential equations. In many of the methods, the signs of α's and β's are mixed. However, the methods satisfying the conditions

$$-\alpha_j \geqq 0,\ j=0,\ 1,\ \ldots,\ k-1,$$
$$\beta_j \geqq 0,\ j=0,\ 1,\ \ldots,\ k$$

are preferable to others because these conditions prevent the cancellation of significant figures during the computations. In this paper, we consider the existence of the implicit LM methods satisfying these conditions, for each of the three types; these types consist of the Adams type, the Milne type, and the Radial type. It is found that the highest orders of such LM methods are 2, 4, and 8, for the Adams, for the Milne, and for the Radial, respectively. In particular, the Adams type includes the A_0- and A-stable methods. For the Milne type, it is found that the methods of order 3, 4 are unstable, and consequently only the one of order 2 is useful. For the Radial type of order from 3 to 5, the optimal parameters are obtained which minimize the round-off error propagations of the methods. The numerical example shows that these optimal methods are more accurate than the Adams-Moulton methods.

1. Introduction

A great number of methods have been derived for solving the initial value problem

$$y'=f(x, y),\ y(x_0)=y_0. \tag{1.1}$$

These methods are classified into the following types of methods:

(1) Runge-Kutta (R-K) methods
(2) Linear multistep (LM) methods

R-K methods are, in general, more accurate and stable, compared with LM methods of same order. Moreover R-K methods are self-starting procedures while LM methods are not so. However, LM methods are superior to R-K methods in that LM methods require a fewer number of function evaluations per step. Most-commonly used LM methods are the Adams-Bashforth (A-B) and the Adams-Moulton (A-M) methods, which are frequently implemented in various steps and various orders (VSVO) mode [1]. Hull et al [2] concluded, from a number of experiments, that the VSVO method based on Adams formula is the best general purpose method, if the function evaluations are relatively expensive.

The k-step Adams method is denoted by

$$y_{n+k}-y_{n+k-1}=h(\beta_k f_{n+k}+\beta_{k-1}f_{n+k-1}+\ldots+\beta_0 f_0), \tag{1.2}$$

$$|\beta_k|+|\beta_0|>0,$$
$$f_j=f(x_j, y_j),$$
$$x_j=x_0+jh.$$

In this formula, the coefficients β's are determined so that the method have maximal order [3]. The signs of the coefficients are, however, mixed for $k>1$, this means that the method (1.2) is vulnerable to the cancellation of significant figures.

In this paper we shall be concerned with the implicit LM method

$$y_{n+k}+\alpha_{k-1}y_{n+k-1}+\ldots+\alpha_0 y_n =h(\beta_k f_{n+k}+\ldots+\beta_0 f_n), \tag{1.3}$$

with the following properties:

$$-\alpha_j \geqq 0,\quad j=0, 1, \ldots, k-1, \tag{1.4}$$

$$\beta_j \geqq 0,\quad j=0, 1, \ldots, k-1, \beta_k>0. \tag{1.5}$$

We say that the method (1.3) is weakly nonnegative method (WNM) if only the conditions (1.4) is satisfied, and that the method is strongly nonnegative method (SNM) if both of the conditions (1.4) and (1.5) are satisfied. For example, the Adams method for $k>1$ is WNM while Simpson method is SNM. In Sec. 2 we will discuss the stability properties of nonnegative methods. From Sec. 3 to Sec. 5, we will derive the SNM of following types:

(1) k-step Adams type correctors of order $k(k>0)$,
(2) k-step Milne type correctors of order $k(k>1)$,

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(3) k-step Radial correctors [4–5] of order $k+1(k>1)$.

2. Stabilities of Nonnegative Methods

In this section we discuss the zero-stability of WNM and the relative stability of SNM. To discuss the stabilities of the LM method (1.3), we define the two polynomials $\rho(\zeta)$ and $\sigma(\zeta)$ in the usual way:

$$\rho(\zeta)=\zeta^k+\alpha_{k-1}\zeta^{k-1}+\ldots+\alpha_0,$$
$$\sigma(\zeta)=\beta_k\zeta^k+\beta_{k-1}\zeta^{k-1}+\ldots+\beta_0. \tag{2.1}$$

Here we assume that the method (1.3) is consistent, i.e., the polynomials associated with the method satisfy the conditions

$$\rho(1)=0, \quad \rho'(1)=\sigma(1). \tag{2.2}$$

The method is said to be zero-stable if it is stable, as $h\to 0$[6]. This condition is equivalent in that no zero of $\rho(\zeta)$ has modulus greater than one and every zero of modulus one is simple [6]. The next Theorem shows that if the consistent LM method is WNM then the method is zero-stable.

Theorem 1.
Assume that the LM method is consistent, and that the polynomials ρ and σ have no common factors. Then the method is zero-stable, if it is WNM.

Proof
For the proof we use a well known result [7] that the magnitudes of the zeros of $\rho(\zeta)$ are no greater than the only real positive zero of the auxiliary polynomial

$$\tilde{\rho}(\zeta)=\zeta^k-|\alpha_{k-1}|\zeta^{k-1}-|\alpha_{k-2}|\zeta^{k-2}-\ldots-|\alpha_0|. \tag{2.3}$$

If the condition (1.4) holds, then the polynomial $\tilde{\rho}(\zeta)$ is identical with $\rho(\zeta)$, and consequently $\rho(\zeta)$ has the only real positive zero $\zeta=1$. This means that all the zeros of $\rho(\zeta)$ satisfy

$$|\zeta|\leqq 1 \tag{2.4}$$

Next we show that any zero of ρ of modulus 1, if they exist, cannot be multiple. Let $\omega(=\exp(\sqrt{-1}\theta)$ be any zero of ρ located on the complex unit circle. Then, it follows, from (1.4), that

$$\begin{aligned}0&=|\rho(\omega)|\\&=|\omega^k||1+\alpha_{k-1}\omega^{-1}+\alpha_{k-2}\omega^{-2}+\ldots+\alpha_0\omega^{-k}|\\&\geqq 1-|\alpha_{k-1}\omega^{-1}|-|\alpha_{k-2}\omega^{-2}|-\ldots-|\alpha_0|\\&=1+\alpha_{k-1}+\alpha_{k-2}+\ldots+\alpha_0\\&=\rho(1)=0\end{aligned} \tag{2.5}$$

which means that

$$\arg \alpha_{k-j}\omega^{-j}\equiv\pi \pmod{2\pi},$$

for all j satisfying $\alpha_{k-j}<0$. Since $\arg\alpha_{k-j}\equiv\pi \pmod{2\pi}$, we have

$$\alpha_{k-j}\omega^{-j}=\alpha_{k-j}. \tag{2.6}$$

Because of that the relation (2.6) is valid even if $\alpha_{k-j}=0$, this relation is valid for all j. From the (2.2) and (2.6), it follows that

$$\begin{aligned}\rho'(\omega)&=k\omega^{k-1}+(k-1)\alpha_{k-1}\omega^{k-2}+\ldots+\alpha_1\\&=\omega^{k-1}(k+(k-1)\alpha_{k-1}\omega^{-1}+\ldots+\alpha_1\omega^{-k+1})\\&=\omega^{k-1}(k+(k-1)\alpha_{k-1}+\ldots+\alpha_1)\\&=\omega^{k-1}\rho'(1)\\&=\omega^{k-1}\sigma(1).\end{aligned} \tag{2.7}$$

Using the assumption that ρ and σ has no common zeros, we can conclude that $\rho'(\omega)\neq 0$, implying that none of the zeros of ρ located on the unit circle should be multiple.

Q.E.D.

Next we discuss the relative stability of the nonnegative method. The LM method (1.3) is said to be relatively stable for a given complex z if each of zeros of the polynomial

$$\pi(\zeta;z)=\rho(\zeta)-z\sigma(\zeta) \tag{2.8}$$

satisfies

$$|\zeta_j|<|\zeta_1|,\quad j=2,3,\ldots,k-1, \tag{2.9}$$

where ζ_1 is a zero which approaches the principal zero of $\rho(\zeta)$, as $z\to 0$, i.e.,

$$\lim_{z\to 0}\zeta_1=1. \tag{2.10}$$

For the relative stability of the LM method Hull and Newbery [5] gave the following theorem:

Theorem 2. (Hull and Newbery [5])
If we attempt to solve the test equation

$$y'=\lambda y,\quad \lambda>0, \tag{2.11}$$

by the LM method (1.3), then the conditions

$$z\beta_k<1, \tag{2.12}$$
$$z\beta_i>\alpha_i,\quad i=0,1,\ldots,k-1, \tag{2.13}$$
$$z=h\lambda$$

guarantee the relative stability.

From this Theorem, the following Theorem is easily derived:

Theorem 3.
Let the method (1.3) be SNM, then it has relative stability for small enough h unless

$$\alpha_i=\beta_i=0,\qquad \text{for some } i.$$

Above results indicate that SNM is superior to the others in the sense that, during the computation, it prevents not only the loss of significant figures by cancellation but also the growth of the round-off error.

3. Adams type SNM Correctors

In this section we derive the k-step Adams type SNM of order k. We call the method (1.3) Adams type, if the first polynomial $\rho(\zeta)$ associated with the method is of the form

$$\rho(\zeta)=\zeta^k-\zeta^{k-1}, \quad k\geqq 1. \tag{3.1}$$

For the k-step Adams type corrector of order k, Rodabaugh and Thompson [8] proved that A_0-stable method (see [11]) exists for $k\leqq 4$ by using the result of Hall [9]. Feinberg [10] also derived the same result in a elegant way.

To find the k-step Adams type SNM correctors, we put

$$\begin{aligned}\rho(\zeta)&=\zeta^k R(t),\\ \sigma(\zeta)&=\zeta^k S(t),\\ t&=1-\zeta^{-1},\end{aligned} \tag{3.2}$$

then from (3.1),

$$R(t)=t. \tag{3.3}$$

Henrici [3] proved that the method (ρ, σ) has order k if and only if the expansion

$$-\frac{R(t)}{\log(1-t)}-S(t)=c_k t^k+\ldots \tag{3.4}$$

holds, where c_k is a constant independent of t. As is shown in [3], since the function $-t/\log(1-t)$ is expanded into the series

$$-\frac{t}{\log(1-t)}=\gamma_0^*+\gamma_1^* t+\ldots, \tag{3.5}$$

$$\gamma_j^*=(-1)^j\int_{-1}^{0}\binom{-s}{j}\mathrm{d}s, \quad j=0, 1, \ldots, \tag{3.6}$$

in order that the method has order k, $S(t)$ should be of the form

$$S(t)=\gamma_0^*+\gamma_1^* t+\ldots+\gamma_{k-1}^* t^{k-1}+at^k, \tag{3.7}$$

where a is an arbitrary constant. It should be noted that if $a=\gamma_k^*$ then the method (ρ, σ) is k-step Adams type corrector of order $k+1$, i.e., k-step A-M method, which satisfies only the weakly nonnegative condition.

Next we determine the coefficients β's from (3.7). To do this we first determine the second polynomial $\sigma(\zeta)$. Substituting the series (3.7) into (3.2), we have

$$\begin{aligned}\sigma(\zeta)&=\zeta^k\left[\sum_{i=0}^{k}\gamma_i^*(1-1/\zeta)^i+(a-\gamma_k^*)(1-1/\zeta)^k\right]\\ &=\sigma^*(\zeta)+(a-\gamma_k^*)(\zeta-1)^k,\end{aligned} \tag{3.8}$$

where

$$\sigma^*(\zeta)=\beta_k^*\zeta^k+\beta_{k-1}^*\zeta^{k-1}+\ldots+\beta_0^*,$$

$$\beta_{k-1}^*=(-1)^i\sum_{j=i}^{k}\binom{j}{i}\gamma_j^*, \quad i=0, 1, \ldots, k. \tag{3.10}$$

Note that $\sigma^*(\zeta)$ is the second polynomial of the k-step A-M method. From these relations, we find

$$\beta_{k-i}=\beta_{k-i}^*+(-1)^i\binom{k}{i}(a-\gamma_k^*), \quad i=0, 1, \ldots, k. \tag{3.11}$$

One can see, from the above expression, that if

$$\begin{aligned}L&=\max_{i=\text{even}}\left\{\gamma_k^*-\binom{k}{i}^{-1}\beta_{k-i}^*\right\}\\ &\leqq\min_{i=\text{odd}}\left\{\gamma_k^*+\binom{k}{i}^{-1}\beta_{k-i}^*\right\}=U,\end{aligned} \tag{3.12}$$

then the free parameter a which makes $\beta_j (j=0, 1, \ldots, k)$ nonnegative exists in the interval $[L, U]$.

$$A_i^{(k)}=\gamma_k^*+(-1)^{i+1}\binom{k}{i}^{-1}\beta_{k-i}^*, \quad i=0, 1, \ldots, k \tag{3.13}$$

then the inequality (3.12) can be rewritten as

$$\max_{i=\text{even}} A_i^{(k)}\leqq\min_{i=\text{odd}} A_i^{(k)}. \tag{3.14}$$

The following Lemma indicates the properties of $A_i^{(k)}$:

Lemma 1.
(i) $A_0^{(k)}<0$, $k=1, 2, \ldots,$
(ii) $A_i^{(k)}>0$, $i=1, 2, \ldots, k-1, k>1,$
(iii) $A_k^{(k)}=0$, $k=1, 2, \ldots,$
(iv) For $i>0$, $A_i^{(k)}$ is monotone decreasing as a function of i.

Proof
(i) Substituting (3.10) into (3.13), we have

$$A_i^{(k)}=-\binom{k}{i}^{-1}\sum_{j=i}^{k-1}\binom{j}{i}\gamma_j^*, \quad i=0, 1, \ldots, k-1. \tag{3.15}$$

From this expression and from the results given by Henrici [3],

$$A_0^{(k)}=-\sum_{j=0}^{k-1}\gamma_j^*=-\gamma_{k-1}, \tag{3.16}$$

where γ_j is a positive constant given by

$$\begin{aligned}r_j&=(-1)^j\int_0^1\binom{-s}{j}\mathrm{d}s\\ &=\int_0^1\frac{s(s+1)\ldots(s+j-1)}{j!}\mathrm{d}s, \quad j\geqq 0.\end{aligned} \tag{3.17}$$

The positiveness of γ_j, $j\geqq 0$, means that $A_0^{(k)}<0$.
(ii) It follows, from (3.6), that γ_j^* can be expressed by

$$r_j^*=\int_{-1}^{0}\frac{s(s+1)\ldots(s+j-1)}{j!}\mathrm{d}s, \quad j=1, 2, \ldots \tag{3.18}$$

From this one can see easily that $\gamma_j^*<0$. Therefore the

assertion $A_k^{(k)}>0$, $(i=1, 2, \ldots, k-1)$ is obtained.
(iii) Using (3.10) and (3.13), we can easily obtain

$$A_k^{(k)}=\gamma_k^*+(-1)^{k+1}\beta_0^* \\ =\gamma_k^*+(-1)^{2k+1}\gamma_k^* \\ =0. \qquad (3.19)$$

(iv) Using (3.10) and (3.13) again, we have

$$A_{i+1}^{(k)}-A_i^{(k)}=(-1)^i\left[\binom{k}{i+1}^{-1}\beta_{k-i-1}^*+\binom{k}{i}^{-1}\beta_{k-i}^*\right] \\ =\sum_{j=i}^{k}\frac{j!(k-i-1)!}{k!(j-i)!}(k-j)\gamma_j^*, \\ i=1, 2, \ldots, k-1. \qquad (3.20)$$

Since $\gamma_j^*<0$ for $j>0$, the assertion $A_{i+1}^{(k)}-A_i^{(k)}<0$ is established.

Q.E.D.

From this Lemma, the following result for L and U is derived:
(i) $k=1$

$$L=A_0^{(1)}=-1, \\ U=A_1^{(1)}=0,$$

(ii) $k=2$

$$L=A_2^{(2)}=0, \\ U=A_1^{(2)}=1/4,$$

(iii) $k=\text{even}>2$

$$A_{k-1}^{(k)}=U<L=A_2^{(k)},$$

(iv) $k=\text{odd}>1$

$$A_k^{(k)}=U<L=A_2^{(k)}.$$

Thus, we have proved the following Theorem:

Theorem 3.
The k-step Adams type SNM corrector families of order k exist only for $k=1$, 2, and the families are

A1: $y_{n+1}=y_n+h[(1+a)f_{n+1}-af_n]$, $\quad -1<a\leqq 0$, (3.20)

error constant: $C_2=-a-1/2$,

and

A2: $y_{n+2}=y_{n+1}+h[(1/2+a)f_{n+2}+(1/2-2a)f_{n+1}+af_n]$, $\quad 0\leqq a\leqq 1/4$, (3.21)

error constant: $C_3=-1/12-a$.

The resulting family A1 is the well-known "θ-method", and is A-stable for $a\geqq -1/2$ [6]. When $a=-1/2$, the method is just the trapezoidal rule. In this family, the trapezoidal rule is optimal because of that the order of the method increases to 2, and that the coefficients β_1 and β_2 are those which can be expressed exactly in any binary or hexa-decimal floating-point systems.

The family A2 is A_0-stable for $a\geqq 0$ [8]. In the range of a in which the methods are SNM, the error constant takes minimum in absolute value at $a=0$. Since the method corresponding to $a=0$ is trapezoidal rule, after all, also in this family, trapezoidal rule is optimal.

4. Milne Type SNM Correctors

In this section we derive the k-step Milne type SNM correctors of order k. We call the method Milne type, if the first polynomial $\rho(\zeta)$ associated with the method is

$$\rho(\zeta)=\zeta^k-\zeta^{k-2}, \quad k\geqq 2. \qquad (4.1)$$

As in the case of Adams type, the coefficients β's of the Milne type can be expressed by

$$\beta_{k-i}=\beta_{k-i}^*+(-1)^i\binom{k}{i}(a-\kappa_k^*), \qquad (4.2)$$

where a is a free parameter, and β_{k-i}^* is the coefficient of the generalized Milne-Simpson method [3]. The coefficient β_{k-i}^* is given by

$$\beta_{k-i}^*=(-1)^i\sum_{j=i}^{k}\binom{j}{i}\kappa_j^*, \qquad (4.3)$$

where κ_j^* is defined by

$$\kappa_j^*=(-1)^j\int_{-2}^{0}\binom{-s}{j}\mathrm{d}s, \quad j=0, 1, \ldots, \qquad (4.4)$$

and has the following properties:

$$\kappa_3^*=0, \\ \kappa_j^*<0, \quad j>3, \qquad (4.5)$$

$$\kappa_0^*+\kappa_1^*+\ldots+\kappa_j^*=\kappa_j, \quad j=0, 1, \ldots \qquad (4.6)$$

$$\kappa_j=(-1)^j\int_{-1}^{1}\binom{-s}{j}\mathrm{d}s, \quad j=0, 1, \ldots, \qquad (4.7)$$

$$\kappa_1=0, \\ \kappa_j>0, \quad j\neq 1. \qquad (4.8)$$

It follows from (4.2) and (4.3) that if the inequality

$$L=\max_{i=\text{even}}\left\{\kappa_k^*-\binom{k}{i}^{-1}\beta_{k-i}^*\right\} \\ \leqq\min_{i=\text{odd}}\left\{\kappa_k^*+\binom{k}{i}^{-1}\beta_{k-i}^*\right\}=U \qquad (4.9)$$

holds, then the coefficients β's of the method are all non-negative, for any a in the interval $[L, U]$. We find the range of k in which the inequality (4.9) is valid. We first set

$$M_i^{(k)}=\kappa_k^*+(-1)^{i+1}\binom{k}{i}^{-1}\beta_{k-i}^*, \quad i=0, 1, \ldots, k. \qquad (4.10)$$

Then the following Lemma holds for $M_i^{(k)}$:

Lemma 2.
(i) $M_k^{(k)}=0$, $\quad k=2, 3, \ldots,$
(ii) $M_0^{(k)}=0$, $\quad k=2,$

$$M_0^{(k)}<0, \quad k>2,$$

(iii) For $k>4$, and for i satisfying $k-1 \geqq i \geqq 4$,

$$M_{i+1}^{(k)}-M_i^{(k)}<0,$$

i.e., $M_i^{(k)}$ is monotone decreasing as a function of i.

Proof

(i) We immediately see from (4.3) that

$$\beta_0^*=(-1)^k \kappa_k^*,$$

and consequently the assertion holds.

(ii) From (4.3), (4.10), and the property (4.6), we have

$$M_0^{(k)}=-\sum_{j=0}^{k-1} \kappa_j^*=-\kappa_{k-1}.$$

This means that

$$M_0^{(k)}=0, \quad \text{for} \quad k=2, \qquad <0, \quad \text{for} \quad k>2.$$

(iii) As in the case of Adams type, we have

$$M_{i+1}^{(k)}-M_i^{(k)}=\sum_{j=i}^{k-1} \frac{j!(k-i-1)!}{k!(j-i-1)!}(k-j)\kappa_j^*, \tag{4.11}$$

and, applying the property (4.5) to this relation, we have

$$M_{i+1}^{(k)}-M_i^{(k)}<0,$$

for $k>4$, $i \geqq 4$.

Q.E.D.

From the property (iii), we immediately see that

$$L \geqq M_{2j}^{(k)}>M_{2j+1}^{(k)} \geqq U$$

for any $j \geqq 2$ and $k>4$. This means that the Milne type SNM does not exist for $k>4$. However, whether or not the SNM exists for $k \leqq 4$ is not clear from this Lemma. Therefore, to clarify this we calculate L and U practically for $k \leqq 4$.

Let $k=2$, then

$$L=\max\{M_0^{(2)}, M_2^{(2)}\}=0,$$
$$U=M_1^{(2)}=-\kappa_1^*/2=1.$$

Consequently the SNM family exists, and the family is the following:

$$\text{M2: } y_{n+2}=y_n+h\{af_{n+2}+2(1-a)f_{n+1}+af_n\}, \quad 0 \leqq a \leqq 1, \tag{4.12}$$

error constant: $C_3=1/3-a$.

For $a=1/3$ this family is just the Simpson method. By the way, this family of the methods has a spurious zero of modulus 1, i.e., $\zeta=-1$. If we solve the equation

$$y'=Ay, \quad A<0,$$

by one of the methods, parastic oscillations in the numerical solution would increase exponentialy, unless the growth parameter is positive (see [3]). This parameter, say λ, for the zero $|\zeta|=1$ is defined by

$$\lambda=\frac{\sigma(\zeta)}{\zeta\rho'(\zeta)}. \tag{4.13}$$

Using this formula, we have for the family M2

$$\lambda=2a-1. \tag{4.14}$$

Therefore the free parameter a should be kept in the interval

$$1/2<a, \tag{4.15}$$

in order that the methods are numerically stable. After all the family M2 is useful only for $1/2<a \leqq 1$.

Next, let $k=3$, then we have

$$L=\max\{M_0^{(3)}, M_2^{(3)}\}=M_2^{(3)}=-1/9,$$
$$U=\min\{M_1^{(3)}, M_3^{(3)}\}=M_3^{(3)}=0. \tag{4.16}$$

Therefore, 3-step SNM family exists, and the family is the following:

$$\text{M3: } y_{n+3}=y_{n+1}+h\{(1/3+a)f_{n+3}+(4/3-3a)f_{n+2} +(1/3+3a)f_{n+1}-af_n\}, \quad -1/9 \leqq a \leqq 0, \tag{4.17}$$

error constant: $C_4=-a$.

The growth parameter for this family is given by

$$\lambda=4a-1/3, \tag{4.18}$$

and consequently λ is positive in the interval

$$1/12<a. \tag{4.19}$$

Because this interval contradicts the one given by (4.17), no stable SNM exists in the family M3.

Finally, for $k=4$, we have

$$L=\max\{M_0^{(4)}, M_2^{(4)}, M_4^{(4)}\}=0,$$
$$U=\min\{M_1^{(4)}, M_3^{(4)}\}=0. \tag{4.20}$$

Therefore, only $a=0$ is permitted and then the method is Simpson's rule

$$y_{n+4}=y_{n+2}+(h/3)\{f_{n+4}+4f_{n+3}+f_{n+2}\}.$$

This method is included in the family M2, and is unstable [3].

After all we have proved the following Theorem:

Theorem 4.

The k-step Milne type SNM corrector families of order k exist only for $k=2$, 3, and the families are M2 and M3.

5. Radial SNM Correctors

In the previous sections, we derived the Adams and the Milne type SNM families of order $\leqq 4$, and showed that the stable SNM families of order >2 do not exist. In practice, however, the methods of lower order are not so useful but those of middle order are most frequently used. Therefore, we derive the stable SNM correctors of middle order.

Hull and Newbery [4], [5] have presented a series of correctors. In each of the correctors, the moduli of the spurious zeros of $\rho(\zeta)$ are taken to be free. According to the manner in which the zeros are located on the complex plane, these formulas are termed a Westward, an East-West, and a Radial formula. In these formulas, the free parameters, i.e., the moduli of spurious zeros, were used to minimize the size of truncation errors or to improve the stability characteristics.

Among these formulas, the Radial methods are WNM as long as they are zero-stable. Therefore, we shall be concerned with the k-step ($k>1$) Radial method of order $k+1$, and search the optimal free parameter experimentally which makes the method SNM and minimize the round-off error propagation. The zeros of $\rho(\zeta)$ of the k-step Radial method are located on the complex plane in a "radial" manner, i.e.,

$$\zeta_1=1,$$
$$\zeta_j=r\cdot\exp\left(\frac{2\pi(j-1)}{k}\sqrt{-1}\right),\quad j=2,3,\ldots,k. \tag{5.1}$$

From this, the coefficients α's are uniquely determined and given by

$$\alpha_j=-(1-r)r^{k-j-1},\quad j=1,2,\ldots,k-1,$$
$$\alpha_0=-r^{k-1}. \tag{5.2}$$

One can see easily from (5.2) that the method is WNM if $0\leqq r\leqq 1$. Note that the method is the A-M if $r=0$ and the Newton-Cotes type if $r=1$.

Here we determine the ranges for r in which the methods are SNM. To do this we express the coefficients β's by r explicitly. In general, k-step LM methods of order $k+1$ are derived so that the methods are exact, if the solution of (1.1) is a polynomial of degree $k+1$. This is done using the polynomial which interpolates $f(x,y)$ at the points $(x_0,f_0),\ldots,(x_k,f_k)$. Such a polynomial $P(x)$ is given by

$$P(x)=\sum_{j=0}^{k}f_jL_j(s),\quad x=x_0+sh, \tag{5.3}$$

where $L_j(s)$ is a Lagrangian interpolation polynomial and is given by

$$L_j(s)=\frac{(-1)^{k-j}}{j!(k-j)!}s(s-1)\ldots(s-j+1)$$
$$\times(s-j-1)\ldots(s-k),\quad j=0,1,\ldots,k \tag{5.4}$$

Using the polynomials $L_j(s)$, $(j=0,1,\ldots,k)$, β's can be represented by

$$\beta_j=\sum_{m=0}^{k}\alpha_m\int_0^m L_j(s)\,ds,\quad j=0,1,\ldots,k. \tag{5.5}$$

Substituting (5.2) into the above, we have the polynomial in r which represents β_j.

$$\beta_j=\sum_{m=0}^{k-1}r^m\int_{k-m-1}^{k-m}L_j(s)\,ds,\quad j=0,1,\ldots,k. \tag{5.6}$$

The error constant C_{k+2} of the method is also represented by the polynomial in r, using the relation [6]

$$C_{p+1}=\frac{1}{(p+1)!}(\alpha_1+2^{p+1}\alpha_2+\ldots+k^{p+1}\alpha_k)$$
$$-\frac{1}{p!}(\beta_1+2^p\beta_2+\ldots+k^p\beta_k), \tag{5.7}$$

where $p=k+1$, $\alpha_k=1$.

The coefficients of these polynomials are listed in Table 1 for $k=2$, 3, 4 (a more detailed list is found in [12]). One can find the range for r in which $\beta_j\geqq 0$ for all j, using the polynomial (5.6). However, it is difficult to calculate the range analytically for large k, because β_j is a polynomial of degree $k-1$. Therefore, we determine the range numerically by a root finder of algebraic equations. The result is shown in Table 2. In calculating these ranges, it is found that the Radial method cannot be SNM for $k=8$, 9.

Table 2 Range $[u, v]$ for r in which k-step Radial method is SNM.

k	u	v
2	0.200	1
3	0.275	1
4	0.437	1
5	0.546	1
6	0.781	1
7	0.795	1
8	none	

Table 1 Cefficients and error constant of k-step Radial Method.

$k=2$	$\alpha_1=-(1-r)$, $\alpha_0=r$ $\beta_2=(5-r)/12$, $\beta_1=(8+8r)/12$, $\beta_0=(-1+5r)/12$ $C_4=(-1+r)/24$
$k=3$	$\alpha_2=-(1-r)$, $\alpha_1=-(1-r)r$, $\alpha_0=-r^2$ $\beta_3=(9-r+r^2)/24$, $\beta_2=(19+13r-5r^2)/24$, $\beta_1=(-5+13r+19r^2)/24$, $\beta_0=(1-r+9r^2)/24$ $C_5=(-19+11r-19r^2)/720$
$k=4$	$\alpha_3=-(1-r)$, $\alpha_2=-(1-r)r$, $\alpha_1=-(1-r)r^2$, $\alpha_0=-r^3$ $\beta_4=(251-19r+11r^2-19r^3)/720$, $\beta_3=(646+346r-74r^2+106r^3)/720$, $\beta_2=(-264+456r+456r^2-264r^3)/720$ $\beta_1=(106-74r+346r^2+646r^3)/720$, $\beta_0=(-19+11r-19r^2+251r^3)/720$ $C_6=(-27+11r-11r^2+27r^3)/1440$

To find the optimal r in the ranges of Table 2, we performe numerical experiments. The equation to be integrated is

$$y' = -4y + \sin 4x,$$
$$y(0) = 1, \tag{5.8}$$
$$y(x) = \frac{\sqrt{2}}{8} \sin\left(4x - \frac{\pi}{4}\right) + \frac{9}{8} \exp(-4x),$$

and the methods to be used are the A-B-Radial predictor-corrector pairs in PECE mode. We calculated the round-off and truncation errors for $k=2$, 3, 4 at $x=4.125$, and the results are shown in Table 3 ~ 5. All calculations were made on a MELCOM-COSMO 700S computer, which has a hexa-deimal mantissa of 6-digit length.

We can see from each Table the magnitude of round-off error is relatively small at $r=0.5$; it takes the minimum for $k=2$, 3 and the second minimum for $k=4$. This is due to the fact that, when $r=0.5$, the methods are SNM and moreover the coefficients α's are all simple values represented by the reciprocals of 2's power. For example, if $k=4$, then $\alpha_3=-1/2$, $\alpha_2=-1/4$, $\alpha_1=-1/8$, $\alpha_0=-1/8$; these values can be expressed exactly on any binary or hexa-decimal floating-point systems. On the binary systems the probability that these coefficients incur the round-off errors in multiplications is 0, while on the hexa-decimal systems it is not 0 but considerably small.

On the other hand, the magnitude of the truncation errors decreases as r increases but at $r=1$ it grows extremely. This is due to the fact that if $r=1$, i.e., if all spurious zeros are located on the unit circle, then at least one of the growth parameters is necessarily negative (see [3], Theorem 5.16). One can deduce qualitatively from this that the absolute stability region of the method is smaller in the neighbour of $r=1$.

In view of the above discussions, the author recommend $r=0.5$ as the optimal parameter for $k=2$, 3, 4. It should be noted that, for each of the Radial families, the method corresponding to $r=0.5$ improves the accuracy of the A-M method (the method corresponding to $r=0$), in spite of that the α's of the Radial method for $r=0.5$ is slightly complex, compared with those of the A-M method. If we put $r=0.5$, the following methods are obtained:

$$\text{R2: } y_{n+2} = \frac{1}{2} y_{n+1} + \frac{1}{2} y_n + \frac{h}{8}(3f_{n+2} + 8f_{n+1} + f_n) \tag{5.9}$$

$$C_4 = -\frac{1}{48}$$

$$\text{R3: } y_{n+3} = \frac{1}{2} y_{n+1} + \frac{1}{4} y_{n+1} + \frac{1}{4} y_n + \frac{h}{96}$$
$$\times (35f_{n+3} + 97f_{n+2} + 25f_{n+1} + 11f_n) \tag{5.10}$$

$$C_5 = -\frac{73}{2880}$$

Table 3 Round-off and truncation errors of Radial method for $k=2$ and $h=2^{-5}$.

16*r	round-off	truncation
0	−2.134E-07	1.167E-06
1	−4.207E-07	1.035E-06
2	−4.960E-07	9.168E-07
3	−4.075E-07	8.133E-07
4	−3.580E-07	7.192E-07
5	−3.351E-07	6.367E-07
6	−3.461E-07	5.620E-07
7	−3.455E-07	4.943E-07
8	−2.037E-07	4.308E-07
9	−3.528E-07	3.750E-07
10	−2.982E-07	3.227E-07
11	−3.448E-07	2.741E-07
12	−2.798E-07	2.294E-07
13	−3.460E-07	1.880E-07
14	−3.364E-07	1.490E-07
15	−2.713E-07	1.132E-07
16	−4.186E-07	−8.164E-04

Table 4 Round-off and truncation errors of Radial method for $k=3$ and $h=2^{-5}$.

16*r	round-off	truncation
0	−2.829E-07	−4.506E-08
1	−4.318E-07	−4.145E-08
2	−4.466E-07	−3.784E-08
3	−3.601E-07	−3.493E-08
4	−2.435E-07	−3.238E-08
5	−3.353E-07	−2.997E-08
6	−2.483E-07	−2.754E-08
7	−2.309E-07	−2.636E-08
8	−1.279E-07	−2.504E-08
9	−1.809E-07	−2.417E-08
10	−2.271E-07	−2.359E-08
11	−2.906E-07	−2.317E-08
12	−2.659E-07	−2.201E-08
13	−2.687E-07	−2.178E-08
14	−2.756E-07	−2.164E-08
15	−2.454E-07	−2.157E-08
16	−1.035E-05	−1.968E-06

Table 5 Round-off and truncation errors of Radial method for $k=4$ and $h=2^{-6}$.

16*r	round-off	truncation
0	−8.845E-08	−1.092E-07
1	−2.021E-07	−9.978E-08
2	−1.814E-07	−9.067E-08
3	−1.901E-07	−8.197E-08
4	−1.377E-07	−7.483E-08
5	−1.427E-07	−6.610E-08
6	−9.700E-08	−5.964E-08
7	−8.273E-08	−5.156E-08
8	3.114E-08	−4.621E-08
9	−5.164E-08	−3.794E-08
10	−4.005E-08	−3.463E-08
11	−4.124E-08	−2.971E-08
12	−7.505E-08	−2.198E-08
13	−9.255E-08	−1.938E-08
14	−1.766E-08	−1.558E-08
15	−2.525E-07	−2.004E-08
16	−4.710E-05	−2.255E-05

$$\text{R4: } y_{n+4}=\frac{1}{2}y_{n+3}+\frac{1}{4}y_{n+2}+\frac{1}{8}y_{n+1}+\frac{1}{8}y_n+\frac{h}{384}\times(129f_{n+4}+434f_{n+3}+24f_{n+2}+126f_{n+1}+7f_n) \quad (5.11)$$

$$C_6=-\frac{167}{11520}$$

The absolute stability regions for $r=0$ and $r=0.5$ are shown in Fig. 1~6.

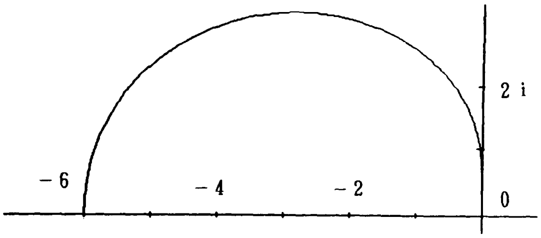

Fig. 1 Absolute stability region of 2-step Radial method for $r=0$.

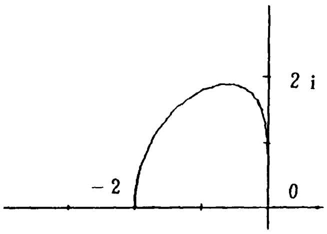

Fig. 2 Absolute stability region of 2-step Radial method for $r=0.5$.

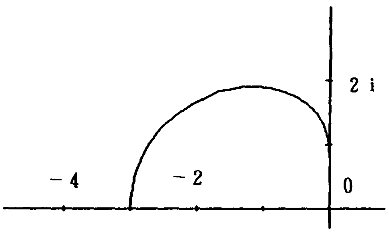

Fig. 3 Absolute stability region of 3-step Radial method for $r=0$.

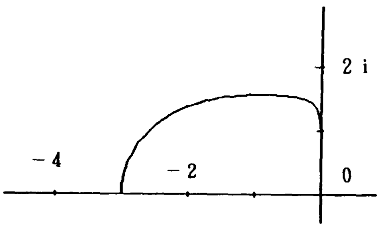

Fig. 4 Absolute stability region of 3-step Radial method for $r=0.5$.

6. Conclusion

We have derived the SNM corrector families of the following types:
(i) Adams type,
(ii) Milne type,
(iii) Radial formula.

It has been proved that the Adams type SNM families including A_0- or A-stable methods exist for $k \leqq 2$, but for $k>2$ the SNM families do not exist at all. For the Milne type, it has been proved that SNM families exist for $k \leqq 3$, but for $k=3$ the family is unstable. On the other hand, for the k-step Radial formulas, it has been shown that the SNM families exist for $k \leqq 7$. In the Radial SNM families of middle order, the optimal parameter which improve the accuracy have been selected. Numerical example shows that these optimal SNM's are more accurate than A-M.

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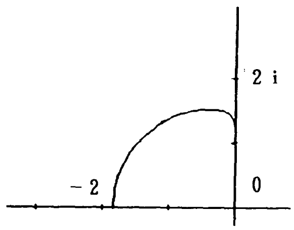

Fig. 5 Absolute stability region of 4-step Radial method for $r=0$.

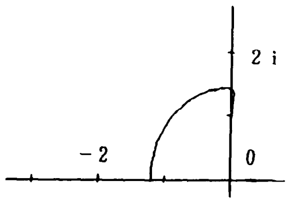

Fig. 6 Absolute stability region of 4-step Radial method for $r=0.5$.

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Appendix

If the differential equation to be integrated is a second order of the form

$$y''=f(x, y), \tag{A.1}$$

then the special kind of LM methods are effective. The general form of such methods is

$$\begin{aligned} &y_{n+k}+\alpha_{k-1}y_{n+k-1}+\ldots+\alpha_0 y_n \\ &\quad =h^2(\beta_k f_{n+k}+\ldots+\beta_0 f_n), \\ &f_j=f(x_j, y_j). \end{aligned} \tag{A.2}$$

In these fomulas, Strömer and Cowell methods are well-known.

In this Appendix, we show that the consistent LM method (A.2) cannot be WNM. To do this, we define the polynomials $\rho(\zeta)$ and $\sigma(\zeta)$ in the usual way.

$$\begin{aligned} &\rho(\zeta)=\zeta^k+\alpha_{k-1}\zeta^{k-1}+\ldots+\alpha_0, \\ &\sigma(\zeta)=\beta_k\zeta^k+\beta_{k-1}\zeta^{k-1}+\ldots+\beta_0. \end{aligned} \tag{A.3}$$

Using these polynomials, the conditions of consistency [6] can be written as

$$\begin{aligned} &\rho(1)=\rho'(1)=0, \\ &\rho''(1)=2\sigma(1). \end{aligned} \tag{A.4}$$

When the first condition of (A.4) holds, one can see easily that

$$\begin{aligned} \rho'(1)&=k\rho(1)-(\alpha_{k-1}+2\alpha_{k-2}+\ldots+k\alpha_0) \\ &=-\alpha_{k-1}-2\alpha_{k-2}-\ldots-k\alpha_0 \\ &=0. \end{aligned} \tag{A.5}$$

If the above relation is valid, either of the following two conditions should be satisfied:

(i) $\alpha_j=0$, for all j,
(ii) The signs of α's are mixed.

Since (i) contradicts $\rho(1)=0$, then (ii) has to be satisfied. Therefore the consistent LM method (A.2) cannot be WNM.