# "Look-ahead" Linear Multistep Methods for Ordinary Differential Equations

## — Introduction of the Method —

Taketomo MITSUI\*

(Received July 13, 2010)

A new class of discrete variable methods for numerical solution of initial-value problem of ordinary differential equations is proposed. This is an extension of linear multistep methods by a "look-ahead" manner. Basically it consists of a pair of predictor and corrector, including the function value at one more step beyond the present step. Starting with the initial idea of the method, its examples, convergence analysis and stability analysis are described. Future works for establishment of the proposed method are also mentioned.

Key words: numerical solution, discrete variable method, predictor-corrector iteration, convergency, stability

#### 1. Introduction

We are concerned with numerical solutions of initial-value problem of ordinary differential equations (ODEs) given by

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x,y) \quad (a \le x \le b), \quad y(a) = y_I. \tag{1}$$

Here the unknown function y is a mapping  $[a, b] \to \mathbb{R}^d$ , the right-hand side function f is  $[a, b] \times \mathbb{R}^d \to \mathbb{R}^d$  and the initial vector  $y_I$  is given in  $\mathbb{R}^d$ .

We are particularly interested in the discrete variable methods (DVMs) with the constant step-size h to generate the approximate solution  $y_n$  of (1) on the step-point  $x_n = a + nh$ . Many existing discrete variable methods like as

Euler method whose numerical scheme is given by  $y_{n+1} = y_n + hf(x_n, y_n)$ ,

Runge-Kutta methods by

$$\begin{cases} Y_i = y_n + h \sum_{j=1}^{i-1} a_{ij} f(x_n + c_j h, Y_j), \\ y_{n+1} = y_n + h \sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i), \end{cases}$$

linear multistep methods by

$$\sum_{i=0}^{k} \alpha_{j} y_{n+j} = h \sum_{i=0}^{k} \beta_{j} f(x_{n+j}, y_{n+j})$$

fall into this category. Note that in the above formulation the parameters  $a_{ij}$ ,  $b_i$ ,  $c_i$ ,  $\alpha_j$ ,  $\beta_j$  characterize a particular method together with the number of stages s in the Runge-Kutta case or with the number of steps k in the linear multistep case. The above-referenced methods are most popular because of their flexible capability for the solution of (1).

We must pay attention to the fact that a method should be 'linear' with respect to the functional values

<sup>\*</sup> Department of Mathematical Sciences, Faculty of Science & Engineering, Doshisha University, Kyoto 610-0394 Phone: +81-774-65-6689, E-mail: tamitsui@mail.doshisha.ac.jp

of y and f to cope with a system of ODEs straightforwardly. Also the step-size h is assumed to be constant, however an adaptive step-size control is significant for practice. A good source of reference to the theory and the practice of numerical solutions of ODEs is the two-volume book by HAIRER et al.<sup>1, 2)</sup>

Numerical analysis is still pursuing a new method in DVM with better performance and higher reliability. The present note proposes a variant of the linear multistep method (LMM) in a look-ahead manner. We call it a "look-ahead" linear multistep method, abbreviated to LALMM, and will describe a general framework of the method in the present note. We remark that the idea "looking ahead" can be seen in a different context<sup>3)</sup>, which is rather concerned with numerical integration of functions, that is, with the case f(x) in place of f(x, y) of (1).

### 2. What is LALMM

Assume that we look for the numerical solution of the (n + k)-th step-point when the back-values  $y_n, y_{n+1}, \ldots, y_{n+k-1}$  and a preassigned *initial guess*  $y_{n+k}^{[0]}$  are available. First, we look ahead for the (n + k + 1)-st step-point by

$$y_{n+k+1}^{[0]} + \alpha_k y_{n+k}^{[0]} + \sum_{i=0}^{k-1} \alpha_i y_{n+i} = h \left( \beta_k f(x_{n+k}, y_{n+k}^{[0]}) + \sum_{i=0}^{k-1} \beta_i f(x_{n+i}, y_{n+i}) \right), (2)$$

which can be regarded as a predictor. Then, correct the look-for value by

$$y_{n+k}^{[1]} + \sum_{i=0}^{k-1} \alpha_i^* y_{n+i} = h\left(\beta_{k+1}^* f(x_{n+k+1}, y_{n+k+1}^{[0]}) + \beta_k^* f(x_{n+k}, y_{n+k}^{[0]}) + \sum_{i=0}^{k-1} \beta_i^* f(x_{n+i}, y_{n+i})\right).$$
(3)

When a (local) convergence attains, i.e., the estimation

$$||y_{n+k}^{[1]} - y_{n+k}^{[0]}|| \le \delta_{TOL}$$

holds for a pre-assigned error tolerance  $\delta_{TOL}$ , we complete the current step and advance to the next step. Otherwise, we replace  $y_{n+k}^{[0]}$  by  $y_{n+k}^{[1]}$  and iterate (2) and (3). Note that generally we assume  $\alpha_j \neq \alpha_j^*, \beta_j \neq \beta_j^*$ . The mechanism of LALMM is shown in Fig.1.

When the current step iteration is completed successfully by m times local iteration, we shift to the right according to the following diagram

$$\begin{array}{lll} \cdots, & (x_{n+k}, y_{n+k}^{[m+1]}), & (x_{n+k+1}, y_{n+k+1}^{[m]}) \\ \rightarrow & (x_{n+k}, y_{n+k}), & (x_{n+k+1}, y_{n+k+1}^{[0]}), & (x_{n+k+2}, y_{n+k+2}) \end{array}$$

by taking  $y_{n+k+1}^{[m]}$  of the current step as the initial guess for the next step and the process is repeated till the end of the integration interval.

In fact several examples have been already known, even though they are not called LALMM. The scheme by USMANI and  $AGARWAL^{4}$ 

$$\begin{cases}
y_{n+2}^{[\ell]} = 5y_n - 4y_{n+1}^{[\ell]} \\
+2h\left\{f(x_n, y_n) + 2f(x_{n+1}, y_{n+1}^{[\ell]})\right\}, \\
y_{n+1}^{[\ell+1]} = y_n + \frac{h}{12}\left\{5f(x_n, y_n) + 8f(x_{n+1}, y_{n+1}^{[\ell]}) \\
-f(x_{n+2}, y_{n+2}^{[\ell]})\right\}
\end{cases} (4)$$

can be regarded as an LALMM of the case for k=1. They claimed that the method possesses a third-order convergence as well as an A-stability. By referring to their work, a new pair of predictor-corrector (PC) was proposed by JACQUES<sup>5</sup>).

$$\begin{cases}
y_{n+2}^{[\ell]} = y_n + 2hf(x_{n+1}, y_{n+1}^{[\ell]}), \\
y_{n+1}^{[\ell+1]} = y_n + \frac{h}{12} \left\{ 5f(x_n, y_n) + 8f(x_{n+1}, y_{n+1}^{[\ell]}) - f(x_{n+2}, y_{n+2}^{[\ell]}) \right\}
\end{cases}$$
(5)

Note that his predictor equation is nothing but the midpoint rule, while his corrector coincides with that of (4). This can be regarded as an LALMM with k = 1, too.

The "extended" backward differentiation formula (EBDF) methods of CASH<sup>6</sup>) can also be seen as an LALMM. More earlier than him, URABE<sup>7</sup>) proposed

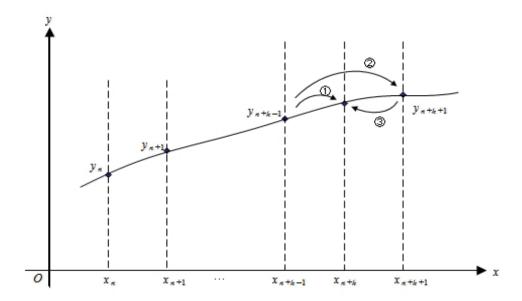


Fig. 1. Mechanism of LALMM.

a new type of DVM. One of its feature is to incorporate the second derivative evaluation of y(x) of (1) given by

$$g(x,y) = \frac{\partial f}{\partial x}(x,y) + \frac{\partial f}{\partial y} \cdot f(x,y).$$

Then Urabe's method can be expressed in the singlestep PC pair given by

$$\begin{cases} y_{n+2}^{[\ell]} = -31y_n + 32y_{n+1}^{[\ell]} \\ -h\left\{14f(x_n, y_n) + 16f(x_{n+1}, y_{n+1}^{[\ell]})\right\} \\ +h^2\left\{-2g(x_n, y_n) + 4g(x_{n+1}, y_{n+1}^{[\ell]})\right\}, \\ y_{n+1}^{[\ell+1]} = y_n \\ +\frac{h}{240}\left\{101f(x_n, y_n) + 128f(x_{n+1}, y_{n+1}^{[\ell]}) \\ +11f(x_{n+2}, y_{n+2}^{[\ell]})\right\} \\ +\frac{h^2}{240}\left\{13g(x_n, y_n) - 40g(x_{n+1}, y_{n+1}^{[\ell]}) \\ -3g(x_{n+2}, y_{n+2}^{[\ell]})\right\}. \end{cases}$$
(6)

The predictor equation is of order 6, while the corrector of order 5, and MITSUI<sup>8)</sup> showed that the method is A-stable. Although the method is often referred as a method utilizing the second derivative, its another aspect lies in the fact that it takes the idea of "lookahead".

More recently, several LALMMs of actually multistep nature have been derived by Yanagiwara's group. For instance, Inamasu et al.  $^{9)}$  gave the schemes in the case k=4 and 5 as follows.

$$\begin{cases} y_{n+5}^{[\ell]} = y_{n+2} + \frac{h}{80} \left( 27f_n - 138f_{n+1} + 312f_{n+2} \right) \\ -198f_{n+3} + 237f(x_{n+4}, y_{n+4}^{[\ell]}) \right), \\ y_{n+4}^{[\ell+1]} = y_{n+3} + \frac{h}{1440} \left( -11f_n + 77f_{n+1} \right) \\ -258f_{n+2} + 1022f_{n+3} \\ +637f(x_{n+4}, y_{n+4}^{[\ell]}) - 27f(x_{n+5}, y_{n+5}^{[\ell]}) \right) \end{cases}$$

$$\begin{cases} y_{n+6}^{[\ell]} = y_{n+3} + \frac{h}{160} \left( -51f_n + 309f_{n+1} \right) \\ -786f_{n+2} + 1134f_{n+3} - 651f_{n+4} \\ +525f(x_{n+5}, y_{n+5}^{[\ell]}) \right), \\ y_{n+5}^{[\ell+1]} = y_{n+3} + \frac{h}{3780} \left( 5f_n - 30f_{n+1} \right) \\ +33f_{n+2} + 1328f_{n+3} + 4863f_{n+4} \\ +1398f(x_{n+5}, y_{n+5}^{[\ell]}) - 37f(x_{n+6}, y_{n+6}^{[\ell]}) \right) \end{cases}$$

$$(8)$$

Here the symbol  $f_{n+j}$  stands for  $f(x_{n+j}, y_{n+j})$ . Note that in their papers they listed the schemes for another context of implementation.

#### 3. Convergency of LALMM

These examples suggest a potential of LALMM in the DVM class. To establish a new class, however, several fundamental issues should be analyzed. The initial steps are for the analysis of convergence and stability of LALMM. We remark that in this stage we will consider an LALMM without the second derivative involved in it.

It is conventional to put the following assumption.

**Assumption 1** In the ODE (1), the function f belongs to  $C^1$ -class, and therefore, satisfies the Lipschitz condition with the constant L. That is, the estimation

$$||f(x,y) - f(x,\widetilde{y})|| \le L||y - \widetilde{y}||$$

holds.

First is a convergency analysis. To this end we formulate an LALMM pair as follows. Assume the predictor equation is

$$y_{n+k+1}^{[\ell]} + \alpha_k y_{n+k}^{[\ell]} + \sum_{i=0}^{k-1} \alpha_i y_{n+i} = h\left(\beta_k f(x_{n+k}, y_{n+k}^{[\ell]}) + \sum_{i=0}^{k-1} \beta_i f_{n+i}\right),$$
(9)

while the corrector

$$y_{n+k}^{[\ell+1]} + \sum_{i=0}^{k-1} \alpha_i^* y_{n+i} = h\left(\beta_{k+1}^* f(x_{n+k+1}, y_{n+k+1}^{[\ell]}) + \beta_k^* f(x_{n+k}, y_{n+k}^{[\ell]}) + \sum_{i=0}^{k-1} \beta_i^* f_{n+i}\right).$$

$$(10)$$

With the pair we associate the modified characteristic polynomials given by

$$\rho(\zeta) = \sum_{i=0}^{k} \alpha_i \zeta^i, \ \sigma(\zeta) = \sum_{i=0}^{k} \beta_i \zeta^i,$$

$$\rho^*(\zeta) = \zeta^k + \sum_{i=0}^{k-1} \alpha_i^* \zeta^i, \ \sigma^*(\zeta) = \sum_{i=0}^{k} \beta_i^* \zeta^i.$$
(11)

Then, by denoting the shift operator with the reference step-size h by S, the predictor and corrector equations

are expressed with

$$\left\{S^{k+1} + \rho(S)\right\} y_n = h\sigma(S)f_n \tag{12}$$

and

$$\rho^*(S)y_n = h\left\{\beta_{k+1}^* S^{k+1} + \sigma^*(S)\right\} f_n, \qquad (13)$$

respectively. We assume a sufficiently smooth solution y(x) of (1).

**Definition 1** Predictor is said to be accurate of order p when it satisfies

$$\{S^{k+1} + \rho(S)\} y(x) - h\sigma(S)y'(x) = Ch^{p+1} + O(h^{p+2}).$$

Corrector is said to be accurate of order q when

$$\rho^*(S)y(x) - h\left\{\beta_{k+1}^* S^{k+1} + \sigma^*(S)\right\} y'(x)$$
  
=  $\widetilde{C}h^{q+1} + O(h^{q+2}).$ 

Here, the constants C and  $\widetilde{C}$  may depend on the IVP and x but does not on h.

We will call a predictor or a corrector is consistent when it is accurate of more than first order. A preliminary power series expansion with respect to h for the predictor eq.

$$y(x + (k+1)h) + \alpha_k y(x + kh)$$

$$+ \sum_{i=0}^{k-1} \alpha_i y(x + ih) - h \sum_{i=0}^{k} \beta_i y'(x + ih)$$

$$= y(x) + (k+1)hy'(x) + \alpha_k (y(x) + khy'(x))$$

$$+ \sum_{i=0}^{k-1} \alpha_i (y(x) + ihy'(x)) - h \sum_{i=0}^{k} \beta_i y'(x) + O(h^2)$$

$$= \left(1 + \alpha_k + \sum_{i=0}^{k-1} \alpha_i\right) y(x)$$

$$+ h \left\{(k+1) + k\alpha_k + \sum_{i=0}^{k-1} i\alpha_i - \sum_{i=0}^{k} \beta_k\right\} y'(x)$$

$$+ O(h^2)$$

leads to the condition that the predictor is consistent iff

$$1 + \alpha_k + \sum_{i=0}^{k-1} \alpha_i = 0$$

and

$$(k+1) + k\alpha_k + \sum_{i=0}^{k-1} i\alpha_i - \sum_{i=0}^{k} \beta_k = 0.$$

This is equivalent to

$$1 + \rho(1) = 0$$
 and  $k + 1 + \rho'(1) - \sigma(1) = 0$ . (14)

Similarly, the condition that the corrector is consistent is

$$1 + \sum_{i=0}^{k-1} \alpha_i^* = 0 \quad \text{and} \quad k + \sum_{i=0}^{k} \alpha_i^* - \beta_{k+1}^* - \sum_{i=0}^{k} \beta_i^* = 0,$$

or, equivalently

$$\rho^*(1) = 0$$
 and  $\rho^{*'}(1) - \beta_{k+1}^* - \sigma^*(1) = 0.$  (15)

Let us confirm the consistency conditions for the abovereferenced schemes. For Usmani-Agarwal's (4) (k=1)we can easily derive

$$\begin{split} & \rho(\zeta) = 4\zeta - 5, \ \sigma(\zeta) = 4\zeta + 2, \\ & \rho^*(\zeta) = \zeta - 1, \ \sigma^*(\zeta) = \frac{8}{12}\zeta + \frac{5}{12} \ \text{and} \ \beta_2^* = -\frac{1}{12}. \end{split}$$

Consequently the conditions (14) and (15) obviously hold. Similarly Jacques' (5) has

$$\rho(\zeta) = -1, \ \sigma(\zeta) = 2\zeta,$$

$$\rho^*(\zeta) = \zeta - 1, \ \sigma^*(\zeta) = \frac{8}{12}\zeta + \frac{5}{12} \text{ and } \beta_2^* = -\frac{1}{12},$$
and enjoys the same conditions.

The scheme (7), which corresponds to k = 4, has the modified characteristic polynomials

$$\begin{cases} \rho(\zeta) = -\zeta^2, \\ \sigma(\zeta) = \frac{1}{80} \left( 27 - 138\zeta + 312\zeta^2 - 198\zeta^3 + 237\zeta^4 \right), \\ \rho^*(\zeta) = \zeta^4 - \zeta^3, \\ \sigma^*(\zeta) = \frac{1}{1440} \left( -11 + 77\zeta - 258\zeta^2 + 1022\zeta^3 + 637\zeta^4 \right) \end{cases}$$
(16)

and the coefficient  $\beta_5^* = -\frac{27}{1440}$ . Thus simple calculations confirm the consistency conditions.

The scheme (8), which corresponds to k=5, has the modified characteristic polynomials

$$\begin{cases}
\rho(\zeta) = -\zeta^3, \\
\sigma(\zeta) = \frac{1}{160} \left( -51 + 309\zeta - 786\zeta^2 + 1134\zeta^3 -651\zeta^4 + 525\zeta^5 \right), \\
\rho^*(\zeta) = \zeta^5 - \zeta^3, \\
\sigma^*(\zeta) = \frac{1}{3780} \left( 5 - 30\zeta + 33\zeta^2 + 1328\zeta^3 +4863\zeta^4 + 1398\zeta^5 \right)
\end{cases}$$
(17)

and the coefficient  $\beta_6^* = -\frac{37}{3780}$ . Again simple calculations confirm the consistency conditions.

Next we assume that the correction-to-convergence mode is taken for the LALMM. Consequently the numerical solution satisfies the identities

$$\left\{ S^{k+1} + \rho(S) \right\} y_n = h \sigma(S) f_n,$$

$$\rho^*(S) y_n = h \left\{ \beta_{k+1}^* S^{k+1} + \sigma^*(S) \right\} f_n$$

On the other hand the exact solution satisfies

$$\begin{cases} \left\{ S^{k+1} + \rho(S) \right\} y(x_n) = h\sigma(S) f(x_n, y(x_n)) + T_n, \\ \rho^*(S) y(x_n) = h \left\{ \beta_{k+1}^* S^{k+1} + \sigma^*(S) \right\} f(x_n, y(x_n)) + \\ \widetilde{T}_n, \end{cases}$$
(18)

where  $T_n$  and  $\widetilde{T}_n$  denote the local truncation errors of the predictor and of the corrector, respectively. Further we suppose the predictor and the corrector are consistent and let  $e_n$  denote the local error at  $x_n$ , i.e.,  $e_n = y(x_n) - y_n$ . We will derive a difference equation which is satisfied by the local truncation error (LTE).

From the predictor equation we have

$$\begin{split} e_{n+k+1} + \alpha_k e_{n+k} + \sum_{i=0}^{k-1} \alpha_i e_{n+1} \\ &= h \bigg\{ \beta_k (f(x_{n+k}, y(x_{n+k})) - f(x_{n+k}, y_{n+k})) \\ &+ \sum_{i=0}^{k-1} \beta_i (f(x_{n+i}, y(x_{n+i})) - f(x_{n+i}, y_{n+i})) \bigg\} \\ &+ T_n, \end{split}$$

which, by introducing the Jacobian matrix  $f_{y,n+i}$  of f with respect to y evaluated at a certain intermediate point, can be written by

$$e_{n+k+1} + \alpha_k e_{n+k} + \sum_{i=0}^{k-1} \alpha_i e_{n+1}$$

$$= h \left\{ \beta_k f_{y,n+k} e_{n+k} + \sum_{i=0}^{k-1} \beta_i f_{y,n+i} e_{n+i} \right\} + T_n.$$

Thus we arrive at the difference equation

$$\{S^{k+1} + \rho(S)\} e_n = h\sigma(S) f_{y,n} e_n + T_n.$$
 (19)

Similarly, the corrector equation derives

$$\rho^*(S)e_n = h\left(\beta_{k+1}^* S^{k+1} + \sigma^*(S)\right) f_{y,n} e_n + \widetilde{T}_n.$$
 (20)

Substituting the former (19) into the latter (20) yields

$$\rho^*(S)e_n = h^2 \beta_{k+1}^* f_{y,n+k+1} \sigma(S) f_{y,n} e_n$$

$$+ h \left\{ -\beta_{k+1}^* f_{y,n+k+1} \rho(S) + \sigma^*(S) f_{y,n} \right\} e_n$$

$$+ \tilde{T}_n + h T_n.$$

Its rearrangement reads

$$\begin{aligned}
& \left(I + h \left(\alpha_{k} \beta_{k+1}^{*} f_{y,n+k+1} - \beta_{k}^{*} f_{y,n+k}\right) \\
& - h^{2} \beta_{k} \beta_{k+1}^{*} f_{y,n+k} f_{y,n+k+1}\right) e_{n+k} \\
&= \sum_{i=0}^{k-1} \left(-\alpha_{i}^{*} - h \beta_{k+1}^{*} \alpha_{i} + h \beta_{i} f_{y,n+i} \\
& + h^{2} \beta_{k+1}^{*} \beta_{i} f_{y,n+k+1} f_{y,n+i}\right) e_{n+i} \\
& + \widetilde{T}_{n} + h T_{n},
\end{aligned} \tag{21}$$

which is nothing but a recurrence relation of LTE.

To show the convergence of LALMM, we need several assumptions.

**Assumption 2** The predictor is consistent but less accurate than the corrector by order one, that is,  $p = q - 1 \ge 1$ .

The above assumption means that there is a certain positive constant K satisfying  $\|\widetilde{T}_n\| + h\|T_n\| = Kh^{q+1}$ .

**Assumption 3** For a certain  $\ell$  between 0 to (k-1),  $\alpha_{\ell}^* = 1$  holds and the other  $\alpha_i^*$ 's vanish.

Note that this is a technical assumption, and, unfortunately, excludes Cash's EBDF methods from our analysis. Further we introduce the following constants.

$$a = |\alpha_k \beta_{k+1}^*|, \quad b = |\beta_k \beta_{k+1}^*|,$$
  
$$\beta = \max_{i=0,\dots,k} (|\beta_i^*| + |\beta_{k+1}^* \alpha_i|) \quad \text{and} \quad \gamma = \max_{i=0,\dots,k} |\beta_{k+1}^* \beta_i|$$

Then we can see for sufficiently small h the coefficient matrix in the left-hand side of (21) is invertible, and arrive at the key inequality

$$||e_{n+k}|| \leq \frac{1 + \beta hL + \gamma h^2 L^2}{1 - ahL - bh^2 L^2} ||e_{n+\ell}|| + \frac{hL(\beta L + \gamma hL)}{1 - ahL - bh^2 L^2} \sum_{i=0, i \neq \ell}^{k-1} ||e_{n+i}|| + \frac{1}{1 - ahL - bh^2 L^2} Kh^{q+1}.$$
 (22)

Here the index  $\ell$  is that which is referred to in Assumption 3. Note that the common denominator  $1 - ahL - bh^2L^2$  can be bounded below for sufficiently small h and that the second term in the right-hand side is always a summation at most over fixed k with the multiplication factor h. Therefore, due to the conventional error analysis, we obtain our main theorem by summing up the above results.

**Theorem 1** Assume that the following conditions hold.

- (1) The predictor and the corrector are consistent.
- (2) The corrector is of order q.
- (3) For a certain  $\ell$   $\alpha_{\ell}^* = -1$  holds and other  $\alpha^*$ 's
- (4) The correction-to-convergence mode is employed.

Then, the method is convergent of order q for sufficiently small h even if the predictor is of order q-1.

Let us see how the theorem works for the schemes which are listed in the previous section. Table 1 shows the constants, the index and the local truncation error terms which feature the convergence of individual scheme. Note that in the row for  $T_n$  and  $\widetilde{T}_n$  the higher derivative  $y_n^{(m)}$  or  $\overline{y}_n^{(m)}$  may refer to a different x-value lying in the integration interval.

### 4. Stability of LALMM

Stability analysis of LALMM runs as follows. When the PC pair of LALMM is applied to the linear test equation

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \lambda y, \qquad \lambda \in \mathbb{C}, \quad \Re \lambda < 0 \tag{23}$$

	(4)	(5)	(7)	(8)
k	1	1	4	5
$\ell$	(none)	(none)	3	3
a	$\frac{1}{3}$	0	0	0
b	$\frac{1}{3}$	$\frac{1}{6}$	$\frac{711}{12800}$	$\frac{37}{1152}$
β	1	$\frac{1}{6}$	$\frac{19}{96}$	$\frac{13}{36}$
γ	$\frac{1}{3}$	$\frac{1}{6}$	$\frac{117}{1600}$	$\frac{11}{1600}$
$T_n$	$-\frac{1}{6}h^4y_n^{(4)}$	$\frac{1}{3}h^3y_n^{(3)}$	$\frac{51}{160}h^6y_n^{(6)}$	$\frac{137}{448}h^7y_n^{(7)}$
$\widetilde{T}_n$	$-\frac{1}{12}h^4\overline{y}_n^{(4)}$	$-\frac{1}{12}h^4\overline{y}_n^{(4)}$	$\frac{27}{604800}h^7\overline{y}_n^{(7)}$	$\frac{1}{756}h^8\overline{y}_n^{(8)}$
order of	3	3	6	7
convergence				

Table 1. Convergence features .

with a fixed positive step-size h, it yields

$$\begin{split} y_{n+k+1}^{[0]} + \alpha_k y_{n+k}^{[0]} + \sum_{i=0}^{k-1} \alpha_i y_{n+i} \\ &= z \left( \beta_k y_{n+k}^{[0]} + \sum_{i=0}^{k-1} \beta_i y_{n+i} \right), \\ y_{n+k}^{[1]} + \sum_{i=0}^{k-1} \alpha_i^* y_{n+i} \\ &= z \left( \beta_{k+1}^* y_{n+k+1}^{[0]} + \beta_k^* y_{n+k}^{[0]} + \sum_{i=0}^{k-1} \beta_i^* y_{n+i} \right) \end{split}$$

with  $z=\lambda h.$  Deleting  $y_{n+k+1}^{[0]}$  from both equations leads to

$$y_{n+k}^{[1]} + \sum_{i=0}^{k-1} \alpha_i^* y_{n+i}$$

$$= z \left( (-\alpha_k \beta_{k+1}^* + \beta_k^* + \beta_k \beta_{k+1}^* z) y_{n+k}^{[0]} + \sum_{i=0}^{k-1} (-\beta_{k+1}^* \alpha_i + \beta_i^* + \beta_{k+1}^* \beta_i z) y_{n+i} \right).$$
(24)

Equating  $y_{n+k}^{[1]}$  and  $y_{n+k}^{[0]}$  of either side of (24) (this means the correction-to-convergence mode for the PC

pair) brings the linear difference equation

$$\left(1 - z(-\beta_{k+1}^* \alpha_k + \beta_k^*) - z^2 \beta_{k+1}^* \beta_k\right) y_{n+k} 
+ \sum_{i=0}^{k-1} (\alpha_i^* - z(-\beta_{k+1}^* \alpha_i + \beta_i^*) - z^2 \beta_{k+1}^* \beta_i) y_{n+i} = 0,$$
(25)

whose characteristic equation becomes to

$$\rho^*(\zeta) - z\sigma^*(\zeta) + \beta_{k+1}^* z \rho(\zeta) - \beta_{k+1}^* z^2 \sigma(\zeta) = 0$$

by employing the modified characteristic polynomials  $\rho, \sigma, \rho^*$  and  $\sigma^*$ . Therefore we can define the stability polynomial  $\pi(\zeta; z)$  by

$$\pi(\zeta; z) = \rho^*(\zeta) - z\sigma^*(\zeta) + \beta_{k+1}^* z \rho(\zeta) - \beta_{k+1}^* z^2 \sigma(\zeta).$$
(26)

Thus we arrive at the following definition.

**Definition 2** The totality of  $z \in \mathbb{C}$  which gives the roots  $\zeta(z)$  of  $\pi(\zeta;z)$  all being less than unity in magnitude is said to be the region of absolute stability of the

scheme. When the region includes the left half-plane of  $\mathbb{C}$ , the scheme is said to have A-stability.

For Usamani-Agarwal's scheme (4), the modified characteristic polynomials are listed in the previous section. Then we can easily obtain

$$\rho^*(\zeta) - z\sigma^*(\zeta) + \beta_{k+1}^* z \rho(\zeta) - \beta_{k+1}^* z^2 \sigma(\zeta) = \left(1 - z + \frac{1}{3}z^2\right)\zeta - \left(1 - \frac{1}{6}z^2\right),$$

which implies that the set

$$\left\{ z \in \mathbb{C}; \ \left| \frac{1 - z^2/6}{1 - z + z^2/3} \right| < 1 \right\} \tag{27}$$

is the region of absolute stability of the scheme. This rightly coincides with their analysis in their paper<sup>4)</sup>, where they claim the method is A-stable. On the other hand, Jacques' scheme (5) yields

$$\pi(\zeta;z) = \left(1 - \frac{2}{3}z + \frac{1}{6}z^2\right)\zeta - \left(1 + \frac{1}{3}z\right),$$

which leads the region of absolute stability

$$\left\{ z \in \mathbb{C}; \ \left| \frac{1 + z/3}{1 - 2z/3 + z^2/6} \right| < 1 \right\}. \tag{28}$$

Similarly to (27), the root of  $\pi(\zeta; z)$  has singular points  $2 \pm i \sqrt{2}$  lying in the right half-plane and its magnitude on the imaginary axis (z = iy) is less than unity in magnitude except the origin (z = 0). Therefore due to the maximum principle, the scheme is again A-stable and, moreover by the expression of the root, is L-stable.

When k exceeds 1, the stability analysis is getting more difficult due to the nature that the root of the stability polynomial is no longer single. Moreover, since Eq. (26) has the  $z^2$ -term, the conventional methods for the stability analysis of the liner multistep methods are powerless, too. Then, we can apply the following criteria to the analysis.

- Schur criterion
- Routh-Hurwitz criterion

As for a reference, the Schur criterion is described here.

Suppose that  $\phi(\zeta)$  is a complex polynomial of essentially degree n. That is, given

$$\phi(\zeta) = c_n \zeta^n + c_{n-1} \zeta^{n-1} + \dots + c_1 \zeta + c_0, \quad (c_j \in \mathbb{C})$$
 (29)

neither  $c_n$  nor  $c_0$  vanishes. When all the roots of  $\phi(\zeta)$  are less than unity in magnitude, it is called a Schur polynomial. According to the suggestion by LAMBERT<sup>10</sup>, the Routh-Hurwitz criterion is most useful (also refer to HAIRER et al.<sup>1)</sup>). The process is as follows. First, we introduce the transformation  $\zeta \to \xi$  by

$$\xi = \frac{\zeta - 1}{\zeta + 1} \quad \Leftrightarrow \quad \zeta = \frac{1 + \xi}{1 - \xi}$$

which maps the inside of the unit circle  $\{\zeta \in \mathbb{C}; |\zeta| < 1\}$  onto the left half-plane  $\{\xi \in \mathbb{C}: \operatorname{Re} \xi < 0\}$ . Then we define the transformed polynomial  $\Phi(\xi)$  by

$$\Phi(\xi) = (1 - \xi)^n \phi\left(\frac{1 + \xi}{1 - \xi}\right) = p_0 \xi^n + p_1 \xi^{n-1} + \dots + p_n.$$
(30)

Theorem 2 (Routh-Hurwitz) Let  $n \times n$  matrix Q be defined through the coefficients of (30) by

$$Q = \begin{bmatrix} p_1 & p_3 & p_5 & \cdots & p_{2n-1} \\ p_0 & p_2 & p_4 & \cdots & p_{2n-2} \\ 0 & p_1 & p_3 & \cdots & p_{2n-3} \\ 0 & p_0 & p_2 & \cdots & p_{2n-4} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & p_n \end{bmatrix}$$

where  $p_j$  should be taken zero when j > n. The polynomial (30) has all the roots lying in the left half-plane if and only if all leading principal minors of Q be positive.

Note that the condition for the polynomial (30) in Theorem is equivalent to that of (29) being Schur. The criterion can avoid the complex conjugate of  $\zeta$  in (29) which appears in the Schur criterion. It will enable us fully to utilize the properties of analytic function. However, an application of the Routh-Hurwitz criterion will

require a tedious task of algebraic manipulations, which can be carried out with a computer algebra system.

#### 5. Concluding remarks and future works

In this note, we propose "look-ahead" linear multistep methods (LALMMs), a new class of DVM, and give an analysis on their convergency and stability. As explained in the previous sections, LALMM appears to be promising for its good stability as well as its high accuracy when compared with the number of steps.

However, many open problems must be solved in the future. A partial list of such problems is given below.

Mode of local iteration The present description focuses on the mode that the local predictor-corrector iteration is carried out till its convergence attains with a reasonable error tolerance. However, from the practical point of view, it is significant what mode of local iteration can be employed. What happens when we employ a single PC-mode without local convergence by a sufficiently small step-size? The problem will relate with other issues.

Global convergence analysis The problem will be discussed according to the mode of local iteration.

Stability analysis In particular for the case  $k \geq 2$ , a more compact criterion of stability is called for. It will also give a guideline in developing new schemes of LALMM. Another analysis for stability will be required according to the mode of local iteration.

**A-posteriori error estimator** To make LALMM schemes competitive with the conventional methods, their a-posteriori error estimator is inevitable.

Step-size control strategy An adaptive step-size control strategy is also significant for a competi-

tive LALMM scheme. Even in the case of k=1, an LALMM scheme passes over multiple steps. Hence an efficient strategy will be a crucial issue of the method.

Second derivative inclusion An inclusion of the second derivative evaluation may increase the performance of LALMM, as proposed by URABE. In that case, theoretical as well as practical issues listed above will be discussed, too.

Many numerical practices Since a good set of test problems has been compiled by the numerical ODE community, a developed LALMM scheme should be practised through such a set to establish its reliability. Total performance is most significant for a numerical solution of ODEs.

Acknowledgements. The present author is supported by the Grants-in-Aid for Scientific Research (No. 21540153) supplied by Japan Society for the Promotion of Science.

#### References

- E. Hairer, S. P. Nørsett, and G. Wanner, Solving Ordinary Differential Equations I, Nonstiff Problems, Second Revised Edition, Springer-V., Berlin, 1993.
- E. Hairer and G. Wanner, Solving Ordinary Differential Equations II, Stiff and Differential-Algebraic Systems, 2nd revised ed., Springer-V., Berlin, 1996.
- R. Jeltsch, "Integration of iterated integrals by multistep methods", Numer. Math., 21:303–316, 1973.
- R. A. Usmani and R. P. Agarwal, "An A-stable extended trapezoidal rule for the integration of ordinary differential equations", Comput. & Math. with Appls., 11:1183–1191, 1985.

- I. B. Jacques, "Extended one-step methods for the numerical solutions of ordinary differential equations", Intern. J. Computer Math., 29:247–255, 1989.
- 6) J. R. Cash, "On the integration of stiff systems of O.D.E.s using extended backward differentiation formulae", Numer. Math., 34:235–246, 1980.
- M. Urabe, "An implicit one-step method of highorder accuracy for the numerical integration of ordinary differential equations", Numer. Math., 15:151-164, 1970.
- T. Mitsui, "A modified version of Urabe's implicit single-step method", J. Comp. Appl. Math., 20:325–332, 1987.
- Y. Inamasu, Y. Kaneko, and H. Yanagiwara, "On a multistep method", J. Fac. International Studies of Culture, Kyushu Sangyou Univ., (1):179–196, 1994.
- 10) J.D. Lambert, Numerical Methods for Ordinary Differential Systems: The Initial Value Problem, John Wiley and Sons, Chichester, England, 1991.