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Order Barrier for Adams type Linear Multistep Multiderivative Methods with Nonnegative Coefficients

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1 Adams type LMM method

Let consider the initial value problem

$$y'(x) = f(x, y), \quad y(a) = \eta, \quad x \in [0, x_f], \tag{1.1}$$

and consider the Adams type liner multistep multiderivative (LMM) method

$$y_{n+k} = y_{n+k-1} + \sum_{i=0}^{k} \sum_{j=1}^{l} h^j \beta_{ij} f_{n+i}^{(j-1)}, \tag{1.2}$$

for solving eq.(1.1), where

$$\begin{aligned}
&f_i^{(j)} = f^{(j)}(x_i, y_i), \quad j = 0, \cdots, l-1, \\
&x_i = ih, \ i = 0, 1, \cdots, N, \\
&f^{(0)}(x, y) = f(x, y), \\
&f^{(j)}(x, y) = \frac{\mathrm{d}}{\mathrm{d}x} f^{(j-1)}(x, y), \ j = 1, \cdots, l-1.
\end{aligned}$$

We assume that the coefficients β's are subject to the constraints

$$(-1)^{j-1}\beta_{ij} \geq 0, \quad i = 0, \cdots, k-1, \tag{1.3}$$

$$(-1)^{j-1}\beta_{kj} > 0, \tag{1.4}$$

$$j = 1, \cdots, l.$$

The method (1.2) is expected to be numerically accurate since the conditions (1.3) and (1.4), say nonnegative conditions, work reasonably well to prevent the cancellation of significant figures during the computation.

The method is stable for small step-size h since all the extraneous zeros of the first characteristic polynomial $\rho(\zeta)$ associated with the method is 0. Moreover, the method (1.2) is expected to be stable even for large step-size h because the nonnegative condition (1.4) is one of the necessary conditions for the method is being A-stable.

To see this, consider the test equation

$$y' = \lambda y. \tag{1.5}$$

If we solve the eq.(1.5) by the method (1.2) then the stability polynomial of the method is given by

$$\pi(\zeta; z) = \eta_k(z)\zeta^k + \eta_{k-1}(z)\zeta^{k-1} + \cdots + \eta_0(z), \tag{1.6}$$

where $z = h\lambda$, and $\eta_i(z)$ are the polynomials of degree$\leq l$ and given by

$$\begin{aligned}
\eta_i(z) &= -\sum_{j=1}^{l} \beta_{ij} z^j, \quad 0 \leq i < k-1, \\
\eta_{k-1}(z) &= -1 - \sum_{j=1}^{l} \beta_{k-1j} z^j, \\
\eta_k(z) &= 1 - \sum_{j=1}^{l} \beta_{kj} z^j.
\end{aligned}$$

We can easily see that the condition (1.4) constitutes a part of the well-known Routh-Hurwitz criterion[4] that the polynomial $\eta_k(z)$, the leading coefficient of the polynomial $\pi(\zeta; z)$, does not vanish on the left half plane, which is one of the necessary conditions for the LMM method being A-stable [6].

We shall consider the attainable order p_{max} of the Adams type LMM method (1.2) with the nonnegative conditions (1.3) and (1.4). In order to discuss the order of the LMM method, we define the linear difference operator associated with the method (1.2) by

$$\mathcal{L}[y(x);h] = y(x+kh) - y(x+(k-1)h) - \sum_{j=1}^{l}\sum_{i=0}^{k}\beta_{ij}h^j y^{(j)}(x+ih), \quad (1.7)$$

where $y(x)$ is a sufficiently differentiable function on the interval $[0, x_f]$. The method (1.2) is said to be of order p, if and only if, in the power series expansion of the operator

$$\mathcal{L}[y(x);h] = C_0\, y(x) + C_1\, y^{(1)}(x)\, h + C_2\, y^{(2)}(x)\, h^2 + \cdots, \quad (1.8)$$

the following condition holds:

$$C_0 = C_1 = \cdots = C_p = 0,\ C_{p+1} \neq 0.$$

The next theorem gives the order barrier for the method (1.2):

Theorem 1 *The attainable order of the method (1.2) is $l+1$, if the coefficients β's are subject to the nonnegative conditions (1.3) and (1.4).*

Proof. It can be easily shown that the maximal order p_{max} of the Adams type LMM method with the nonnegative conditions is at least $l+1$ since the method given by

$$y_{n+1} = y_n + h\left(\frac{l}{l+1}\,f_{n+1} + \frac{1}{l+1}\,f_n\right) + \sum_{j=2}^{l} h^j(-1)^{j-1}\,\frac{l+1-j}{(l+1)j!}\,f_{n+1}^{(j-1)} \quad (1.9)$$

is of order $l+1$; this method is based on the Padé approximation to e^z of order $l+1$, hence the method is of order $l+1$. Next we show that the method (1.2) cannot be of order$> l+1$ under the nonnegative conditions.

Consider the function $y(x) = (x-k)^r$ as an exact solution of (1.1). Then the jth derivative of the function is given by

$$y^{(j)}(x) = (r)_j\,(x-k)^{r-j},\ j = 1, \cdots, l, \quad (1.10)$$

where

$$(r)_j = \begin{cases} r(r-1)\cdots(r-j+1), & r \geq j, \\ 0, & r < j. \end{cases}$$

If the method is of order p and $r \leq p$, then the numerical solution given by the method (1.2) coincides with the exact solution $y(x) = (x-k)^r$ regardless of the step-size $h > 0$, and therefore we have the following relations:

$$y_i = y(ih) = (ih-k)^r, \tag{1.11}$$

$$f_i^{(j-1)} = f^{(j-1)}(ih, y(ih)) = (r)_j \ (ih-k)^{r-j}, \tag{1.12}$$

$$i = 0, \cdots, N, \ \ j = 1, \cdots, l.$$

Substituting these into (1.2) for $r = 1, \cdots, p$, and taking $h = 1$ and $n = 0$, we have

$$1 = \sum_{j=1}^{l} (r)_j \ \sum_{i=0}^{k} (-1)^{j-1} \beta_{ij} (k-i)^{r-j}, \ \ r = 1, \cdots, p, \tag{1.13}$$

where we define $0^0 = 1$. In particular we have for $r > l$

$$1 = \sum_{i=0}^{k-1} (k-i)^{r-l} \sum_{j=1}^{l} (r)_j \ (-1)^{j-1} \beta_{ij} (k-i)^{l-j}, \ \ r = l+1, \cdots, p. \tag{1.14}$$

We can easily see that at least one of the β's appearing on the right-hand side is nonzero since the left-hand side is not 0. However, if some of the β's in this relation were nonzero then the expression on the right-hand side would be an increasing function of r, but left-hand side is a constant. We can conclude, from the fact, that even if the relation (1.14) holds for some values of r, it cannot be true for more than two values of r. Thus, the relation (1.14) cannot be valid for $r > l+1$, since we have already had an example that the relation (1.14) is valid for $r = l+1$; the relation is valid for $r = l+1$ if the β's are those of the method(1.9). ∎

2 Optimal Adams type LMM method

In this section we show that the Adams type LMM method (1.9) is the optimal formula in the sense that the method minimizes the absolute value of the error constant among the class of the Adams type LMM methods having maximal order p_{max}.

Theorem 2 *Let the Adams type LMM method (1.2) with nonnegative conditions (1.3) and (1.4) be of order* $l+1$. *Then the error constant* C_{l+2} *takes minimum in modulus if*

$$\begin{aligned} \beta_{kj} &= \frac{(-1)^{j-1}(l+1-j)}{(l+1)j!}, \quad j=1,\cdots,l, \\ \beta_{k-11} &= \frac{1}{l+1}, \\ \beta_{ij} &= 0, \qquad\qquad\qquad \text{otherwise,} \end{aligned} \tag{2.1}$$

i.e., the method (1.9) is the optimal.

Proof. The coefficients C_ν in the power series expansion (1.8) for the method (1.2) is given by

$$C_\nu = \frac{1}{\nu!}\{k^\nu - (k-1)^\nu\} + \sum_{j=1}^{\min\{\nu,l\}} \sum_{i=0}^{k} \beta_{ij}\frac{i^{\nu-j}}{(\nu-j)!}, \quad \nu = 1,2,\cdots. \tag{2.2}$$

We must optimize the error constant C_{l+2} under the condition that

$$C_1 = C_2 = \cdots = C_{l+1} = 0, \tag{2.3}$$

since the method is of order $l+1$ by assumption.

The system of the constraints (2.3) together with the nonnegative conditions define a convex subset in $(k+1)l$-dimensional vector space, since the constraints (2.3) are linear in β's. It is well known that a linear objective function defined on a convex subset takes optima at some extreme points of the convex set [3]. In our case extreme points are the points which is expressed by the $(k+1)l$-tuples such that some $kl-1$ components are specified as 0 and the other $l+1$ components are determined so as to satisfy the linear equations (2.3).

In order to get the feasible extreme points, which are the candidates for the optimal solution, we need one more component, say β_{st}, $(1 \le s < k,\ t = 1, \cdots, l)$, to be determined by the equation (2.3), because we have already had l nonzero components β_{kj}, $(j = 1, \cdots, l)$. Solving eq.(2.3) for the variables β_{kj} and β_{st}, we have

$$(-1)^{j-1} j! \beta_{kj} = \begin{cases} 1, & 1 \le j < t, \\ 1 - (-1)^{t-1} \binom{j}{t} (k-s)^{j-t} t! \beta_{st}, & t \le j \le l, \end{cases} \tag{2.4}$$

$$(-1)^{t-1} t! \beta_{st} = (k-s)^{t-l-1} \binom{l+1}{t}^{-1} \tag{2.5}$$

Using these results we have the expression for the error constant C_{l+2}

$$C_{l+2} = \frac{(-1)^l}{(l+2-t)(l+2)!} \{(k-s-1)(l+2)+t\}. \tag{2.6}$$

It is clear that $\mid C_{l+2} \mid$ takes minimum at $s = k-1$ and $t = 1$. Taking $s = k-1$ and $t = 1$ we have the coefficients β's given by eq.(2.1) and the optimum value of C_{l+2}

$$C_{l+2} = \frac{(-1)^l}{(l+2)!(l+1)}. \tag{2.7}$$

This completes the proof of Theorem 2. ∎

As pointed out earlier, the optimal method (1.9) is based on the Padé approximation to e^z. In this case the numerator and the denominator of the approximation function are the polynomials in z of degree 1 and l, respectively. According to the theory of "order stars" the corresponding approximation is A-acceptable for $1 \le l \le 3$, and in particular L-acceptable for $l = 2, 3$ [5], so that the method is A- and L-stable for

$1 \le l \le 3$ and for $l = 2, 3$, respectively.

Corollary *The trapezoidal rule is optimal in the class of the Adams type linear multistep (LM) methods*

$$y_{n+k} = y_{n+k-1} + h(\beta_k f_{n+k} + \cdots + \beta_0 f_n), \tag{2.8}$$

with the nonnegative coefficients

$$\beta_k > 0, \ \ \beta_i \ge 0, \ \ i = 0, \cdots, k-1. \tag{2.9}$$

3 Numerical example

Consider the scalar equation

$$y'(x) = ay(x) + p'(x) - ap(x), \ \ y(0) = p(0), \tag{3.1}$$
$$\text{exact solution}: \ y(x) = p(x),$$

and the Obrechkoff method

$$y_{n+1} = y_n + \frac{h}{2}(f_{n+1} + f_n) - \frac{h^2}{12}(f_{n+1}^{(1)} - f_n^{(1)}), \tag{3.2}$$

as an example of numerical methods for solving eq.(3.1). In solving the equation by the method (3.2) we must solve at each step of the integration the following scalar equation:

$$\begin{aligned} \left(1 - \frac{ah}{2} + \frac{a^2h^2}{12}\right) y_{n+1} &= \left(1 + \frac{ah}{2} + \frac{a^2h^2}{12}\right) y_n \\ &+ \frac{h}{2}(u_{n+1} + u_n) - \frac{h^2}{12}(v_{n+1} - v_n), \end{aligned} \tag{3.3}$$

where

$$u(x) = p'(x) - ap(x),$$
$$v(x) = p''(x) - a^2p(x).$$

Although, in computing this recurrence relation, we must expect a loss of significant figures due to the cancellation in $v_{n+1} - v_n$, this will be usually not a serious problem since the small coefficients $h^2/12$ is being multiplied by $v_{n+1} - v_n$. However, this may not be true in the case that the magnitude of $v(x)$ is so large compared with that of $u(x)$, which may happen, for example, when solving the equation (3.1) having large constant $\mid a \mid$. Let $p(x)$ be

$$p(x) = \sin^6\left(\frac{\pi}{2}x\right),$$

and $a = -100$ in eq.(3.1). In this case the value of $|h^2 v(x)|$ is close to that of $|hu(x)|$ if $x = 1$ and $h = 2^{-10}$; we have $|h^2 v(x)| \approx 9.55 \times 10^{-3}$ and $|hu(x)| \approx 9.77 \times 10^{-2}$. In the situations like this the use of the formula having nonnegative coefficients such as (1.9) will be successful.

Let consider the method

$$y_{n+1} = y_n + \frac{h}{4}(3f_{n+1} + f_n) - \frac{h^2}{4}f_{n+1}^{(1)} + \frac{h^3}{24}f_{n+1}^{(2)}, \tag{3.4}$$

which corresponds to $l = 3$ in (1.9). As stated earlier, the method is of order 4, same with the Obrechekoff method. We shall compare these two methods by the total errors at $x = 1.03125$ for varying step-size. The results for $a = -1$ and $a = -10$ are shown in Fig.1 and 2. It is clear from the figures that the LMM method with nonnegative conditions is superior to the Obrechkoff method.

Next we trace the total errors of the two methods in the cases that round-off errors are dominant over the discretization errors. The results are shown in Fig.3 and 4. The superiority of the method (3.4) is also clear from the figures. These computations have been performed on an ACOS 2020 computer of Computer Center of Tohoku University, and the language used is FORTRAN 77 in double precision mode.

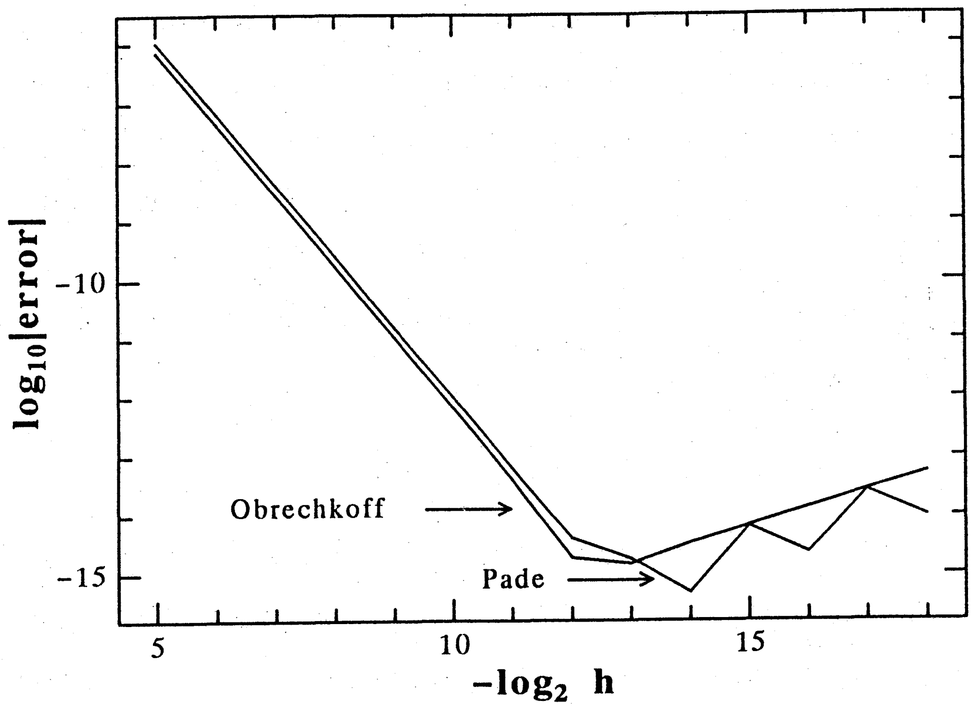

Figure 1. Total errors at $x = 1.03125$ for $a = -1$.

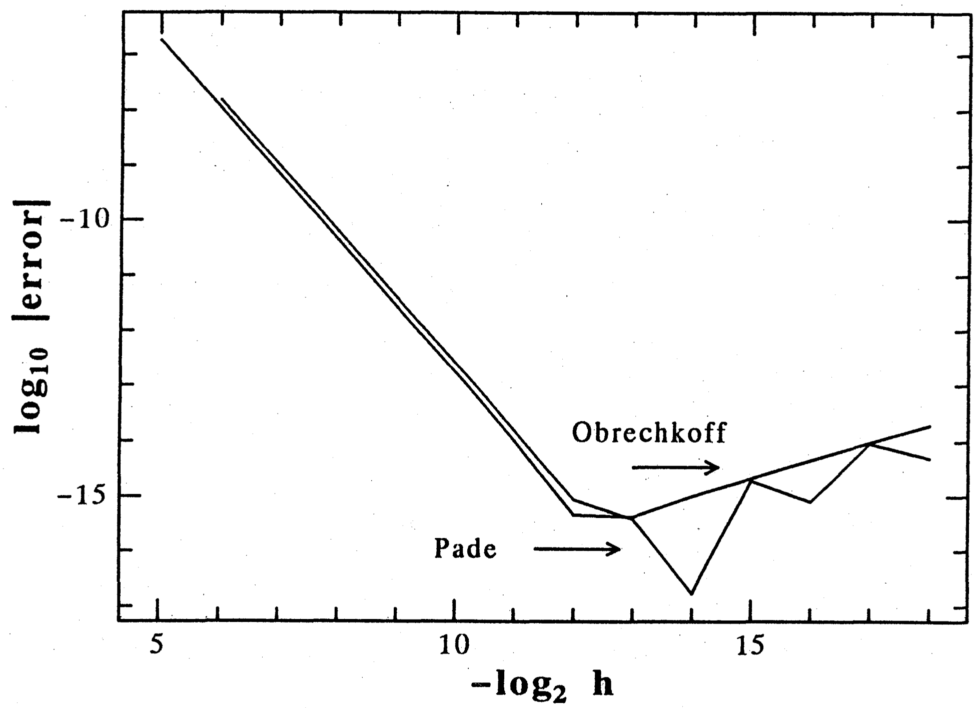

Figure 2. Total errors at $x = 1.03125$ for $a = -10$.

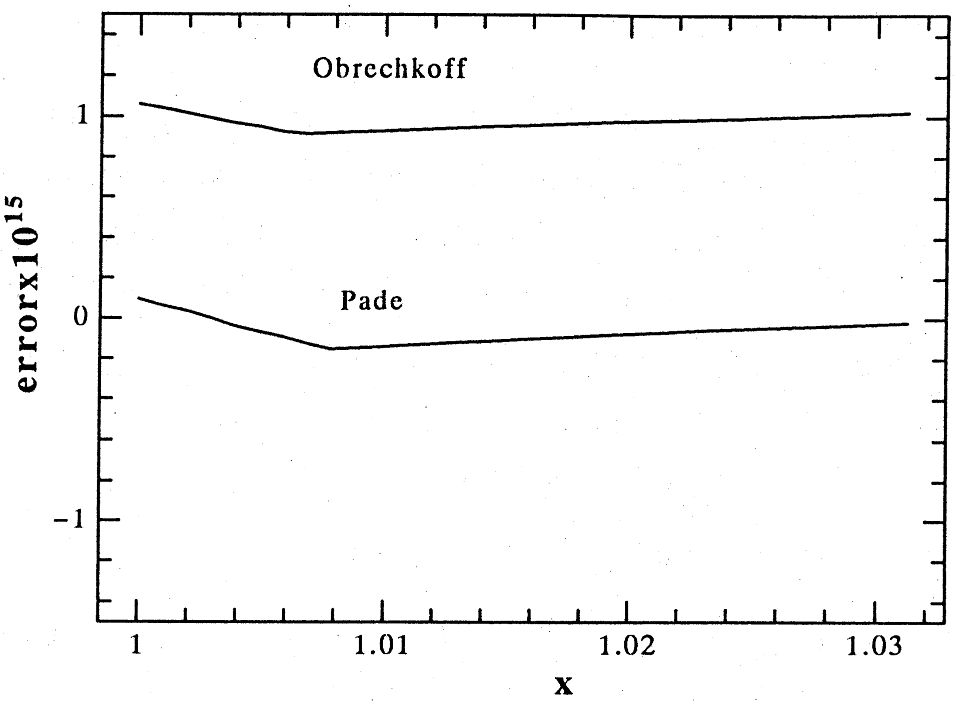

Figure 3. Total error sequences for $a = -1$.

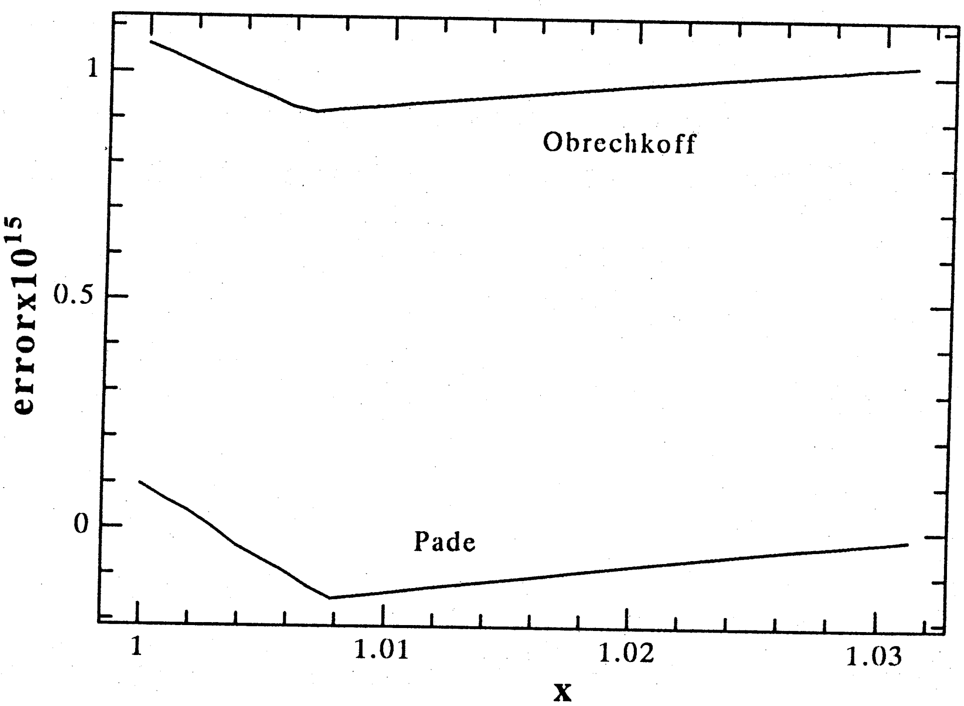

Figure 4. Total error sequences for $a = -10$.

4 Concluding remarks

In this paper we have discussed the order barrier of the Adams type LMM method, and derived some optimal method under the conditions (1.3) and (1.4). However, as discussed in Sec. 3, these conditions are somewhat restrictive in general situations. It is necessary to discuss the order barrier and an optimal method under the less restrictive condition such that

$$\beta_{i1} \geq 0, \quad i = 0, \cdots, k-1,$$
$$(-1)^{j-1}\beta_{kj} > 0, \quad j = 1, \cdots, l,$$

in which the coefficients β_{ij}, ($j = 2, \cdots, l$, $i < k$) are not subject to any constraints.

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5 Appendix

Here we will give a conjecture on the order barrier for the linear multistep method

$$y_{n+k} = -\alpha_{k-1}y_{n+k-1} - \cdots - \alpha_0 y_n + h(\beta_k f_{n+k} + \cdots + \beta_0 f_n), \qquad (5.1)$$

where the coefficients α's and β's are subject to the constraints

$$-\alpha_i \geq 0, \quad i = 0, \cdots, k-1, \qquad (5.2)$$

$$\beta_i \geq 0, \quad i = 0, \cdots, k. \qquad (5.3)$$

We demand, moreover, the LM method(5.1) to be zero-stable. It is well known that no zero-stable k-step LM method can have order exceeding k+2, and that if a zero-stable k-step LM method is of order $k+2$ then the following conditions must be satisfied [1]:

1. The step number k is even.
2. All the zeros of the first characteristic polynomial $\rho(\zeta)$, which is given by

   $$\rho(\zeta) = \zeta^k + \alpha_{k-1}\zeta^{k-1} + \cdots + \alpha_0,$$

   are located on the unit circle.
3. In particular $\zeta = \pm 1$ are the zeros of $\rho(\zeta)$.

It follows, from these conditions, that the characteristic polynomial $\rho(\zeta)$ associated with the method of maximal order has the form

$$\rho(\zeta) = (\zeta^2 - 1)\prod_\nu (\zeta^2 - 2\cos\theta_\nu \zeta + 1), \qquad (5.4)$$

and therefore $\alpha_0 = -1$. Moreover the third of the above conditions leads to

$$\alpha_{k-1} + \cdots + \alpha_1 = 0,$$

implying that

$$\alpha_j = 0, \quad j = 1, \cdots, k-1,$$

since the coefficients $-\alpha$'s are nonnegative. We can conclude, from this, that if the LM method (5.1) with the nonnegative conditions (5.2) and (5.3) has maximal order p_{max} then the method must be the Newton-Cotes type, i.e., the method must be of the form

$$y_{n+k} = y_{n+k-1} + h(\beta_k f_{n+k} + \cdots + \beta_0 f_n). \tag{5.5}$$

According to Davis and Rabinowitz[2], the coefficients β's of the Newton-Cotes type formula of order $k+2$, which is equivalent to the Newton-Cotes type numerical quadrature formula, are given by

$$\beta_i = \frac{(-1)^{k-i}}{i!(k-i)!} \int_0^k t(t-1)\cdots(t-i+1)(t-i)\cdots(t-k)\mathrm{d}t, \qquad i = 0, \cdots, k, \tag{5.6}$$

and these coefficients have the asymptotical property

$$\beta_i = \frac{(-1)^{i-1}k!}{i!(k-i)!k\log^2 k}\left[\frac{1}{i} + \frac{(-1)^k}{k-i}\right]\left[1 + O\left(\frac{1}{\log k}\right)\right], \quad k \to \infty. \tag{5.7}$$

It can be easily seen from eq.(5.7) that the coefficient β_i changes its sign alternatively for sufficiently large k. Using formula (5.6) we can confirm numerically that

- For $k = 2, 4, 6$,

$$\beta_i \geq 0, \quad i = 0, \cdots, k.$$

- But for any even k satisfying $8 \leq k \leq 20$

$$\beta_{\frac{k}{2}}\,\beta_{\frac{k}{2}-1} < 0.$$

Thus, the attainable order p_{max} of the LM method is expected to be 8, if the coefficients α's and β's are subject to the constraints (5.2) and (5.3).