

A Necessary Condition for A -Stability of Multistep Multiderivative Methods

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Abstract. The region of absolute stability of multistep multiderivative methods is studied in a neighborhood of the origin. This leads to a necessary condition for A -stability. For methods where $\rho(\zeta)/(\zeta - 1)$ has no roots of modulus 1 this condition can be checked very easily. For Hermite interpolatory and Adams type methods a necessary condition for A -stability is found which depends only on the error order and the number of derivatives used at (x_{n+k}, y_{n+k}) .

1. Introduction and Results. A multistep method using higher derivatives for solving the initial value problem $y' = f(x, y)$, $y(a) = \eta$ is given by

$$(1) \quad \sum_{i=0}^k \alpha_i y_{n+i} - \sum_{j=1}^l h^j \sum_{i=0}^k \beta_{ji} f^{(j)}(x_{n+i}, y_{n+i}) = 0, \quad n = 0, 1, 2, \dots$$

α_i, β_{ji} are real constants, $\alpha_k \neq 0$, $\sum_{i=0}^k |\beta_{ii}| \neq 0$, $|\alpha_0| + \sum_{j=1}^l |\beta_{j0}| \neq 0$, $x_n = a + nh$, $h > 0$, and

$$f^{(1)}(x, y) = f(x, y);$$

$$f^{(j+1)}(x, y) = \frac{\partial f^{(j)}(x, y)}{\partial x} + f(x, y) \frac{\partial f^{(j)}(x, y)}{\partial y}, \quad j = 1, 2, \dots, l-1.$$

It is well known that the method has order p if

$$(2) \quad \rho(e^z) - \sum_{j=1}^l z^j \sigma_j(e^z) = \sum_{j=p+1}^{\infty} C_j z^j, \quad C_{p+1} \neq 0,$$

where $\rho(\zeta)$ and $\sigma_j(\zeta)$ are the polynomials

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

We shall always assume that the polynomials ρ and σ_j , $j = 1, 2, \dots, l$, have no common factor. The method is convergent if and only if $p \geq 1$ and $\rho(\zeta)$ is a simple von Neumann polynomial; that is, if ζ is a root of $\rho(\zeta)$, then $|\zeta| \leq 1$; and if $|\zeta| = 1$, then it is a simple root (see R. Jeltsch [8]).

If the multistep method (1) is applied to the test equation $y' = \mu y$, $y(0) = 1$, μ complex, then (1) is a linear recurrence relation with constant coefficients. The corresponding characteristic equation is

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$$(3) \quad \rho(\xi) - \sum_{j=1}^l z^j \sigma_j(\xi) = 0, \quad z = \mu h.$$

For each z , (3) has k roots $\xi_i(z)$, $i = 1, 2, \dots, k$. The set $A = \{z \mid |\xi_i(z)| < 1, i = 1, 2, \dots, k\}$ is called the region of absolute stability. Let $\partial A = \bar{A} - A$, where \bar{A} is the closure of A . A method is called A -stable if A contains the whole left-hand plane $\text{Re } z < 0$.

In several articles the boundary ∂A of A has been plotted in order to determine whether a method is A -stable or not, see Brown [1], Enright [4], Jeltsch [7]. However, if all growth parameters λ_j , given by (4), are positive, then ∂A will be extremely close to the imaginary axis for z close to 0. Roundoff errors may defeat the attempt to determine whether ∂A is in a neighborhood of $z = 0$ in $H^+ = \{z \in \mathbb{C} \mid \text{Re } z > 0\}$ or in $H^- = \{z \in \mathbb{C} \mid \text{Re } z < 0\}$. Our results fill this gap. In particular, we shall find a necessary condition for A -stability. It should be noted that a method which violates this condition may still behave numerically almost like an A -stable method even though it is not A -stable. In Section 2 this necessary condition for A -stability is applied to Hermite interpolatory and Adams-type multistep multiderivative methods; and it is found that these cannot be A -stable if the error order p is equal to $2l_k + 1$ modulo 4, where

$$l_k = \begin{cases} 0 & \text{if } \sum_{j=1}^l |\beta_{jk}| = 0, \\ t & \text{if } \sum_{j=t+1}^l |\beta_{jk}| = 0 \text{ and } \beta_{tk} \neq 0. \end{cases}$$

The proofs are given in Section 3.

Let $\xi_j, j = 1, 2, \dots, s$, be the roots of $\rho(\xi)$ with modulus 1. Let us introduce the growth parameters

$$(4) \quad \lambda_j = \sigma_1(\xi_j) / \xi_j \rho'(\xi_j), \quad j = 1, 2, \dots, s,$$

and

$$(5) \quad \mu_j = \frac{1}{\xi_j \rho'(\xi_j)} \left(\sigma_2(\xi_j) + \xi_j \lambda_j \sigma_1'(\xi_j) - \frac{1}{2} \xi_j^2 \lambda_j^2 \rho''(\xi_j) \right), \quad j = 1, 2, \dots, s.$$

Furthermore, let the method have order $p \geq 1$. Then we define recursively

$$(6) \quad c_j = \left(C_j - \sum_{i=1}^{j-p-1} c_{j-i} s_i \right) / s_0, \quad j = p + 1, p + 2, \dots, 2p,$$

where s_0, s_1, \dots, s_{p-1} are given by

$$(7) \quad \sum_{j=1}^l j z^{j-1} \sigma_j(e^z) = \sum_{i=0}^{p-1} s_i z^i + O(z^p).$$

For the disk $\{z \in \mathbb{C} \mid |z| < R\}$ we shall use the symbol $D(R)$.

THEOREM 1. *Let the multistep method of form (1) be convergent, of order $p \geq 1$ and let $\rho(\xi)$ have s roots of modulus 1, $\xi_i, i = 1, 2, \dots, s$, with $\xi_1 = 1$. Let λ_i be real and positive, $i = 1, 2, \dots, s$; and define*

$$\delta = \begin{cases} 1, & s = 1, \\ \min_{j=2,3,\dots,s} \{2 \operatorname{Re} \mu_j - \lambda_j^2\}, & s \geq 2, \end{cases}$$

where λ_j and μ_j are given by (4) and (5), respectively. Assume that one of the conditions (I), (II₁)–(II₄) holds, where

(I) $\delta < 0$.

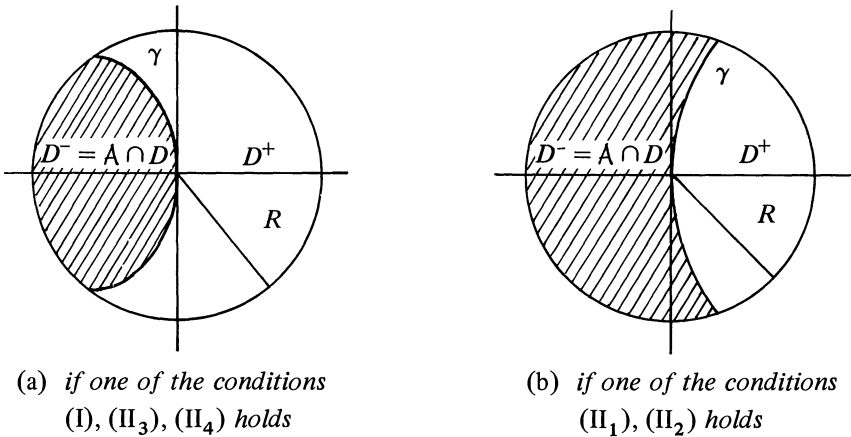
(II₁) $\delta > 0, p$ odd, $c_{p+1}(-1)^{(p+1)/2} > 0$.

(II₂) $\delta > 0, p$ even, $c_{p+2q}(-1)^{(p/2)+q} > 0, c_{p+2j} = 0, j = 1, 2, \dots, q - 1$, for some $q \leq p/2$.

(II₃) $\delta > 0, p$ odd, $c_{p+1}(-1)^{(p+1)/2} < 0$.

The numbers $c_j, j = p + 1, p + 2, \dots, 2p$, are given by (6). Then there exists a disk $D = D(R), R > 0$, such that $\gamma = \partial A \cap D$ is a continuously differentiable curve which intersects the real axis and the imaginary axis only at $z = 0$. The imaginary axis is tangent to γ at $z = 0$. γ divides D in two simply connected regions $D^- = A \cap D$ and $D^+ = D - D^-$, see Figure 1. Moreover, each of the conditions (I), (II₃), (II₄) implies that $D^- \subset H^-$ while each of the conditions (II₁), (II₂) implies that $D^+ - \{0\} \subset H^+$.

FIGURE 1. Absolute stability region in a neighborhood of the origin



Remarks. 1. Using (2) and (7), one finds the explicit formulas

$$(8) \quad C_n = \frac{1}{n!} \sum_{m=0}^k \alpha_m m^n - \sum_{j=1}^{\min\{n, l\}} \frac{1}{(n-j)!} \sum_{m=0}^k \beta_{jm} m^{n-j}, \quad n = p + 1, p + 2, \dots,$$

and

$$(9) \quad s_n = \sum_{j=1}^{\min\{n+1, l\}} \frac{j}{(n+1-j)!} \sum_{m=0}^k \beta_{jm} m^{n+1-j}, \quad n = 0, 1, 2, \dots, p - 1.$$

Moreover, from (6), (7) and (2) follows

$$(10) \quad c_{p+1} = C_{p+1}/\rho'(1) \neq 0$$

and

$$(11) \quad c_{p+2} = \left(C_{p+2} - \frac{C_{p+1}}{\rho'(1)} (\sigma'_1(1) + 2\sigma_2(1)) \right) / \rho'(1).$$

2. Let $s = 1$. If p is odd, then Theorem 1 describes ∂A close to $z = 0$ in all cases since $c_{p+1} \neq 0$. The methods with p even and $c_{p+2j} = 0, j = 1, 2, \dots, p/2$, are not covered by Theorem 1. However, there are only a few methods with this property since one has the following result by Griepentrog [6]. There exists no k -step method of form (1) with $k \geq 2$ and $s = 1$ for which ∂A lies exactly on the imaginary axis in a neighborhood of $z = 0$. Moreover, a one-step method of form (1) with $p \geq 1$ has ∂A on the imaginary axis in a neighborhood of $z = 0$ if and only if $\beta_{j1} = (-1)^{j+1}\beta_{j0}, j = 1, 2, \dots, l$.

THEOREM 2. *It is necessary for a method to be A-stable that all growth parameters are real and nonnegative, $\delta \geq 0$ and either (III) or (IV) holds, where δ is defined as in Theorem 1 and*

$$(III) \quad p \text{ odd, } c_{p+1}(-1)^{(p+1)/2} > 0.$$

$$(IV) \quad p \text{ even, either } c_{p+2j} = 0, j = 1, 2, \dots, p/2, \text{ or } c_{p+2j}(-1)^{(p/2)+q} > 0, \\ c_{p+2j} = 0, j = 1, 2, \dots, q - 1, \text{ for some } q \leq p/2.$$

Remark. This necessary condition for A-stability is very easy to check for $s = 1$. If p is odd, only c_{p+1} has to be calculated. If p is even one finds for most methods that $c_{p+2} \neq 0$; and hence, only c_{p+2} has to be calculated. The following lemma simplifies the problem of determining the sign of c_{p+1} .

LEMMA. *Let the multistep method using higher derivatives be convergent, then $\text{sign } \rho'(1) = \text{sign } \alpha_k$.*

Proof. Since the method is convergent, all roots of $\rho(\xi)$ and $\rho'(\xi)$ lie in the unit disk and hence the lemma holds.

2. Application to Hermite Interpolatory and Adams Type Methods.

Definition 1. A linear multistep method using higher derivatives of the form

$$\sum_{i=0}^k \alpha_i y_{n+i} - \sum_{i=0}^k \sum_{j=1}^{l_i} h^j \beta_{ji} f^{(j)}(x_{n+i}, y_{n+i}) = 0$$

is called Hermite interpolatory if the error order p is at least $\sum_{i=0}^k l_i + k - 1$.

In Jeltsch [9] the following theorem is proved.

THEOREM 3. *Let a set of nonnegative integers l_0, l_1, \dots, l_k with $\max_{i=0,1,\dots,k} l_i = l > 0$ be given. Then there exists a unique Hermite interpolatory multistep method with the given $l_i, \alpha_k \neq 0$ and $\beta_{l_k k} \neq 0$. The error order is $p = \sum_{i=0}^k l_i + k - 1$ and one has*

$$\text{sign } C_{p+1} = (-1)^l \text{sign } \alpha_k.$$

A similar result can be established for Adams-type methods which are defined as follows.

Definition 2. A linear multistep method using higher derivatives is said to be of Adams type if it is of the form

$$y_{n+k} - y_{n+k-1} - \sum_{i=0}^k \sum_{j=1}^{l_i} h^j \beta_{ji} f^{(j)}(x_{n+i}, y_{n+i}) = 0,$$

and its error order p is at least $\sum_{i=0}^k l_i$.

THEOREM 4. *Let a set of nonnegative integers l_0, l_1, \dots, l_k with $\max l_i = l > 0$ be given. Then there exists a unique Adams-type multistep method with the given l_i and $\beta_{l_k k} \neq 0$. The error order is $p = \sum_{i=0}^k l_i$ and one has*

$$\text{sign } C_{p+1} = (-1)^{l_k} \text{sign } \alpha_k.$$

Using Theorems 2, 3, 4 and the Lemma, one then finds immediately the

THEOREM 5. *A convergent linear multistep method using higher derivatives which is of Adams type or Hermite interpolatory cannot be A-stable if the error order p satisfies*

$$p = 2l_k + 1 \pmod{4}.$$

Example 1. Brown's methods are interpolatory with

$$l_0 = l_1 = \dots = l_{k-1} = 0, \quad l_k = l.$$

Hence, the methods are not A-stable if $p = 2l + 1 \pmod{4}$. Especially the methods with $k = 4, l = 2, p = 5; k = 5, l = 3, p = 7$ and $k = 6, l = 4, p = 9$ are not A-stable. The method with $p = 10, k = 7$ and $l = 4$ is not covered by Theorem 5. However, A. H. Sipilä has computed C_{11} and C_{12} using rational arithmetic and it was found that

$$c_{12} = (C_{11}/3\rho'(1))(-4.653007\dots).$$

Hence, by our Lemma and Theorem 3, one has $c_{12}(-1)^{p/2+1} < 0$. Hence, by Theorem 2 this method is not A-stable. Note that in Brown [1] the plots of ∂A lead to the wrong conclusion that these methods are A-stable.

Example 2. Consider the linear one-step methods using higher derivatives which are based on the (r, l) entry of the Padé table of $\exp(x)$, see Jeltsch [8] or Ehle [3, p. 89]. These methods have order $p = r + l$ and are interpolatory. It is known, see Ehle [3], that the methods are A-stable for $r = l, l - 1, l - 2$. From Theorem 5 it follows that the methods are not A-stable for $r = l - 3$. This result has been found by Ehle [3].

Example 3. Enright's second derivative methods are of Adams type with $l_0 = l_1 = \dots = l_{k-1} = 1$ and $l_k = 2$, with order $p = k + 2$, see Enright [4]. Using the Lemma and Theorems 1 and 4, one finds that for $k = 3 \pmod{4}$ the region of absolute stability behaves at the origin as given in Figure 1a and for $k = 5 \pmod{4}$ as given in Figure 1b.

3. Proof of the Results.

Proof of Theorem 1. The algebraic function $\zeta(z)$ which satisfies (3) has k branches $\zeta_j(z)$ with $\zeta_j(0) = \zeta_j, j = 1, 2, \dots, k$. Since $|\zeta_j(0)| < 1$ for $j = s + 1, s + 2, \dots, k$ there exists a $D(R_1), R_1 > 0$ such that $|\zeta_j(z)| < 1$ for all $z \in D(R_1)$,

$j = s + 1, s + 2, \dots, k$. $\zeta_j(0), j = 1, 2, \dots, s$, are simple zeros of $\rho(\zeta)$; and hence, there exists a disk $D(R_2), 0 < R_2 < R_1$, such that the branches $\zeta_j(z)$ are analytic in $D(R_2)$. By the method of undetermined coefficients one finds

$$(12) \quad \zeta_j(z) = \zeta_j(0)(1 + \lambda_j z + \mu_j z^2 + O(z^3)), \quad j = 1, 2, \dots, s;$$

and hence,

$$(13) \quad \left. \frac{d\zeta_j(z)}{dz} \right|_{z=0} = \zeta_j(0)\lambda_j \neq 0, \quad j = 1, 2, \dots, s.$$

Hence, there exists an $R_3, 0 < R_3 < R_2$, such that the mapping $\zeta_j(z): z \rightarrow \zeta = \zeta_j(z)$ is one to one on $z \in D(R_3)$. Moreover, R_3 can be chosen so small that the curves $\gamma^{(j)} = \{z \in D(R_3) \mid |\zeta_j(z)| = 1\}$ are continuously differentiable. Clearly, $\{0\} \in \gamma^{(j)}$ and from (13) it follows that the imaginary axis is tangent to $\gamma^{(j)}$ at $z = 0$. If $i \neq j$, then either $\gamma^{(j)} \cap \gamma^{(i)}$ is a finite set or $\tilde{\gamma}^{(j)} \cap \gamma^{(i)}$ is a continuous curve which contains $z = 0$. Hence, there exists $\tilde{R}, 0 < \tilde{R} < R_3$, such that either $\gamma_j \cap \gamma_i = \{0\}$ or $\gamma_j \equiv \gamma_i$ and $\gamma_j \cap [-\tilde{R}, \tilde{R}] = \{0\}$ for $j = 1, 2, \dots, s$, where $\gamma_j = D(\tilde{R}) \cap \gamma^{(j)}$. Each γ_j separates $D(\tilde{R})$ in the two sets $D_j^- = \{z \in D(\tilde{R}) \mid |\zeta_j(z)| < 1\}$ and $D_j^+ = \{z \in D(\tilde{R}) \mid |\zeta_j(z)| \geq 1\}$. Clearly, $(-\tilde{R}, 0) \subset D_j^-, j = 1, 2, \dots, s$. We distinguish now two cases:

(i) Consider $\zeta_j(z), j = 2, 3, \dots, s$. With $z = iy, y \in (-\tilde{R}, \tilde{R})$, one finds from

$$(14) \quad \begin{aligned} |\zeta_j(iy)| &= |1 - y^2 \operatorname{Re} \mu_j + i(\lambda_j y - y^2 \operatorname{Im} \mu_j) + O(y^3)| \\ &= \operatorname{sqrt}(1 - y^2(2\operatorname{Re} \mu_j - \lambda_j^2) + O(y^3)). \end{aligned}$$

(ii) Consider $\zeta_1(z)$. It is well known, see, e.g. Gear [5] that $\zeta_1(z) - e^z = O(z^{p+1})$. Since $\zeta_1(z)$ is analytic at the origin, we can write

$$(15) \quad \zeta_1(z) = e^z \left(1 - \sum_{j=p+1}^{2p} c_j z^j + O(z^{2p+1}) \right).$$

If one substitutes (15) in (3) and uses (2), one finds easily that $c_j, j = p + 1, p + 2, \dots, 2p$, are determined by (6) and (7). Note that c_j is a real number. Let p be odd. Then $c_{p+1}i^{p+1} = c_{p+1}(-1)^{(p+1)/2}$ is real and nonzero. Hence we find for $z = iy, y$ real,

$$(16) \quad \begin{aligned} |\zeta_1(iy)| &= |e^{iy}| |1 - c_{p+1}i^{p+1}y^{p+1} + O(y^{p+2})| \\ &= \operatorname{sqrt}(1 - 2c_{p+1}(-1)^{(p+1)/2}y^{p+1} + O(y^{p+2})) \quad \text{for } p \text{ odd.} \end{aligned}$$

Let p be even. Then $c_{p+2j}i^{p+2j} = c_{p+2j}(-1)^{(p/2)+j}$ is real for $j = 1, 2, \dots, p/2$. Hence, we find for $z = iy, y$ real

$$(17) \quad \begin{aligned} |\zeta_1(iy)| &= |e^{iy}| \left| 1 - \sum_{j=1}^{p/2} c_{p+2j}i^{p+2j}y^{p+2j} \right. \\ &\quad \left. - i \sum_{j=0}^{(p/2)-1} c_{p+2j+1}i^{p+2j}y^{p+2j+1} + O(y^{2p+1}) \right| \\ &= \operatorname{sqrt} \left(1 - 2 \sum_{j=1}^{p/2} c_{p+2j}(-1)^{(p/2)+j}y^{p+2j} + O(y^{2p+1}) \right) \quad \text{for } p \text{ even.} \end{aligned}$$

Assume now that condition (I) holds. Then it follows from (14) that there exists $R, 0 < R < \tilde{R}$, such that $|\zeta_j(iy)| > 1$ for y real, $0 < |y| < R$ for at least one $j \in \{2, 3, \dots, s\}$. Therefore, $D^- = A \cap D(R) = \bigcap_{j=1}^s D_j^- \cap D(R) \subset H^-$.

If $(II_1), (II_2)$, respectively, hold then by (16), (17) and (14) there exists $R, 0 < R < \tilde{R}$, such that $|\zeta_1(iy)| < 1$ and $|\zeta_j(iy)| < 1, j = 2, 3, \dots, s$, for y real, $0 < |y| < R$. Therefore, $D^+ = \bigcup_{j=1}^s D_j^+ \cap D(R)$ satisfies $D^+ - \{0\} \subset H^+$ since $D_j^+ \cap D(R) - \{0\} \subset H^+$. Similarly, one finds that $(II_3), (II_4)$ imply $D^- \subset H^-$. This completes the proof of Theorem 1.

Proof of Theorem 2. Let $\lambda_j = de^{i\phi}, d > 0, \phi \in (0, 2\pi)$. Clearly,

$$\psi = \frac{3\pi}{2} - \frac{\phi}{2} \in \left(\frac{\pi}{2}, \frac{3\pi}{2}\right) \quad \text{and} \quad \psi + \phi \in \left(\frac{3\pi}{2}, \frac{5\pi}{2}\right).$$

Hence, using (12), one finds

$$|\zeta_j(re^{i\psi})| = |1 + rde^{i(\phi+\psi)} + O(r^2)| > 1$$

for all $r > 0, r$ sufficiently small. Therefore, the method is not A -stable. Let $\lambda_j \geq 0, j = 1, 2, \dots, s$, and $\delta < 0$. From (14) follows immediately that the method is not A -stable. Similarly, using (16) and (17) one finds that (III), (IV) are necessary for A -stability. This establishes Theorem 2.

Proof of Theorem 4. In Jeltsch [9] it is shown that to given nonnegative integers l_0, l_1, \dots, l_k with $\max l_i = l > 0$ there exists a unique Adams-type method with the given $l_i, \beta_{l_k k} \neq 0$ and that the error order $p = \sum_{i=0}^k l_i$. Hence, it remains to show that

$$(18) \quad \text{sign } C_{p+1} = (-1)^{l_k} \text{sign } \alpha_k.$$

To show this we construct the method explicitly. Let $P(x)$ be the interpolation polynomial of degree $\sum_{i=0}^k l_i - 1$ which satisfies

$$P^{(j-1)}(x_i) = y_{n+i}^{(j)} = f^{(j)}(x_{n+i}, y_{n+i}), \quad j = 1, 2, \dots, l_i, i = 0, 1, 2, \dots, k.$$

The multistep method is obtained by setting

$$(19) \quad y_{n+k} - y_{n+k-1} = \int_{x_{n+k-1}}^{x_{n+k}} P(x) dx.$$

To find the error order and C_{p+1} we apply the method given by (19) to a sufficiently smooth function $y(x)$. Clearly,

$$(20) \quad y'(x) - P(x) = f^*(x) \prod_{i=0}^k (x - x_{n+i})^{l_i},$$

where $f^*(x)$ is the generalized divided difference of the function $y'(x)$ on the set

$$S = \underbrace{\{x, x_n, x_n, \dots, x_n\}}_{l_0\text{-times}} \underbrace{\{x_{n+1}, x_{n+1}, \dots, x_{n+1}\}}_{l_1\text{-times}} \underbrace{\{x_{n+2}, \dots, x_{n+k}, x_{n+k}, \dots, x_{n+k}\}}_{l_k\text{-times}}$$

see e.g. Conte and de Boor [2, p. 223]. Hence,

$$\begin{aligned} \int_{x_{n+k-1}}^{x_{n+k}} (y'(x) - P(x)) dx &= \int_{x_{n+k-1}}^{x_{n+k}} f^*(x) \prod_{i=0}^k (x - x_{n+i})^i dx \\ &= f^*(\zeta) \int_{x_{n+k-1}}^{x_{n+k}} \prod_{i=0}^k (x - x_{n+i})^i dx, \end{aligned}$$

since the factor $\prod_{i=0}^k (x - x_{n+i})^i$ does not change sign in the interval $[x_{n+k-1}, x_{n+k}]$; and hence, the second mean value theorem of the integral calculus can be applied, $\zeta \in [x_{n+k-1}, x_{n+k}]$. But $f^*(\zeta) = 1/((p+1)!)y^{(p+1)}(\eta)$, where $\eta \in [x_n, x_{n+k}]$; and hence,

$$(21) \quad \int_{x_{n+k-1}}^{x_{n+k}} (y'(x) - P(x)) dx = Kh^{p+1}y^{(p+1)}(\eta),$$

where

$$(22) \quad K = \frac{1}{(p+1)!} \int_0^1 \prod_{i=0}^k (s+k-1-i)^i ds.$$

Using (21), it is easy to see that the method given by (19) is of error order p and that $C_{p+1} = K$. From (22) follows that $\text{sign } C_{p+1} = (-1)^k$. The proof of Theorem 4 is complete since there exists exactly one Adams-type method.

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