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PRECISELY A(α)-STABLE ONE-LEG MULTISTEP METHODS*

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Abstract.

One-Leg Multistep (OLM) methods for initial value problems in ODEs use a nonlinear multistep formula to compute the solution at the next integration point. This paper shows that there exists an evaluation point t^* which gives an OLM formula more precise than BDF's and (almost) precisely A(α)-stable for a k-step method ($k \leq 6$), and whose stability angle is essentially similar to BDF's. The stability region can be further improved by applying the corrector idea of Klopfenstein.

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1 Introduction.

This paper considers One-Leg Multistep (OLM) methods for the solutions of initial value problems

$$y'(t) = f(t, y(t)) \tag{1.1}$$

on a time interval $[t_0, t_f]$, given initial values $y(t_0) = y_0$. The one-leg multistep formulas (e.g., [2]) are derived from the functional equation

$$p'(t) = f(t, p(t)), \tag{1.2}$$

where p is an approximation of the solution y. In the following, we restrict attention to the cases where the approximation p is a polynomial of degree $\leq k$ that interpolates the points

$$(t_n, y_n), \ldots, (t_{n+k}, y_{n+k}).$$

Hence Equation (1.2), when applied to a specific time t_e, produces an *implicit nonlinear multistep* formula

$$p'(t_e) = f(t_e, p(t_e)) \tag{1.3}$$

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which can be used to approximate the value $y(t_{n+k})$. In the following, we denote these formulas by OLM_k for k steps.

The choice of t_e has a fundamental impact on the accuracy and stability of OLM formulas. Obviously, Equation (1.2) at time t_{n+k} gives a backward differentiation formula (BDF). Moreover, Dahlquist [2] showed that there exists a time t^+ such that the OLM_k formula

$$p'(t^+) = f(t^+, p(t^+)) \tag{1.4}$$

produces a method of order $k+1$. In fact, it can be shown that the OLM_k formula has essentially the same accuracy and stability properties as the k-step Adams–Moulton formula.

This paper considers the stability counterpart of the Dahlquist's accuracy result. It shows that there exists a time t^* such that the OLM_k formula

$$p'(t^*) = f(t^*, p(t^*)) \tag{1.5}$$

produces a method with the following properties:

(1) It is A(α)-stable, its stability angle α is comparable to the one of BDF_k, and its stability region (almost) does not intersect with $\mathbb{C}^+$.
(2) It is of order k and more precise than BDF_k.

In particular, for $k = 2$, the method is precisely A-stable (i.e., its region of absolute stability is precisely the left half-plane) and is as accurate as the Trapezoidal Rule. Assuming a constant step size h, point t is defined in terms of a ratio τ satisfying

$$t = t_n + \tau h.$$

The ratios τ^+ and τ^* defining t^+ and t^* are roots of polynomials that depend only on the number of steps k and can thus be computed once for all for each k. Finally, we also show how to apply the corrector idea from Klopfenstein [6] to OLM formulas. These corrected formulas significantly improve the stability region while only degrading accuracy slightly.

We believe that this result is potentially interesting for several reasons. On the one hand, Lambert ([7, page 231]) argues for precisely A-stable methods which avoid the misleading results which are sometimes produced by L-stable methods and are not easily detected by an automatic code. On the other hand, observe that precisely A-stable methods, e.g., code based on the Trapezoidal Rule, are now finding their way into commercial tools, precisely because the BDFs and their variants are not appropriate for some stiff ODEs [11]. Since OLM methods with the ratio τ^* can be viewed as a generalization of the Trapezoidal Rule, they could thus be of practical interest for some classes of problems.

The rest of the paper characterizes the ratios τ^* as well as the additional parameter arising in the corrected OLM formulas. Section 2 defines the OLM formulas precisely and presents the main tools to carry out the analysis. Section 3 characterizes the ratio τ^*, studies the accuracy and stability of the corresponding OLM formula, and compares it to BDF's. Section 4 shows how to apply the corrector idea from [6] to further improve the stability region.

2 One-Leg Multistep methods.

When the step size is a constant h, the OLM$_k$ formula, for a step from (t_{n+k-1}, y_{n+k-1}) to (t_{n+k}, y_{n+k}), can be written in terms of backward differences as

$$\boxed{p'(t) - f(t, p(t)) = 0} \tag{2.1}$$

where

$$\begin{aligned}
p(t) &= \sum_{j=0}^{k} \zeta_j(\tau)\nabla^j y_{n+k},\\
p'(t) &= \frac{1}{h}\sum_{j=1}^{k} \zeta_j'(\tau)\nabla^j y_{n+k},\\
t &= t_n + \tau h,\\
\zeta_0(\tau) &= 1,\\
\zeta_j(\tau) &= \frac{1}{j!}\prod_{m=0}^{j-1}(\tau + m - k) \quad (1 \le j \le k),\\
\zeta_j'(\tau) &= \zeta_j(\tau)\delta_j(\tau) \quad (1 \le j \le k),\\
\delta_j(\tau) &= \sum_{m=0}^{j-1} \frac{1}{\tau + m - k} \quad (1 \le j \le k).
\end{aligned} \tag{2.2}$$

When $t = t_{n+k}$, OLM$_k$ reduces to BDFk:

$$\sum_{j=1}^{k} \frac{1}{j}\nabla^j y_{n+k} - hf(t_{n+k}, y_{n+k}) = 0. \tag{2.3}$$

Observe that the OLM$_k$ formula is parametrized by the ratio τ and hence it defines a class of OLM$_k$ formulas. In the following, we use OLM$_k(\tau)$ to represent the OLM$_k$ formula for a given τ.

OLM formulas are nonlinear multistep methods because of the term $f(t, p(t))$. Consider the linear form of an OLM formula, i.e., the linear multistep method (LMM)

$$\sum_{j=0}^{k} \alpha_j(\tau) y_{n+j} = h\sum_{j=0}^{k} \beta_j(\tau) f_{n+j}, \tag{2.4}$$

where $(j = 0, \ldots, k)$

$$\begin{aligned}
\alpha_j(\tau) &= \varphi_j'(\tau),\\
\beta_j(\tau) &= \varphi_j(\tau),\\
\varphi_j(\tau) &= \prod_{\substack{m=0\\ m\neq j}}^{k} \frac{\tau - m}{j - m},\\
f_{n+j} &= f(t_{n+j}, y_{n+j}).
\end{aligned} \tag{2.5}$$

We can easily verify that, for all τ, the formula (2.4) is normalized, i.e., $\sum_{j=0}^{k} \beta_j(\tau) = 1$. We now show that

(1) Formulas (2.1) and (2.4) have order at least k;
(2) when either formula (2.1) or (2.4) has order k, the formulas have the same order and the same error constant (i.e., they have the same accuracy);
(3) the formulas (2.1) and (2.4) have the same linear stability.

2.1 Accuracy.

Consider the linear difference operator

$$\mathcal{L}[y(t_n), h] = \sum_{j=0}^{k} \alpha_j(\tau) y(t_{n+j}) - h \sum_{j=0}^{k} \beta_j(\tau) y'(t_{n+j}) \tag{2.6}$$

of the linear multistep method (2.4) and let us associate a difference operator with OLM_k

$$\Phi[y(t_n), h, \tau] = \sum_{j=0}^{k} \alpha_j(\tau) y(t_{n+j}) - hf\left(t, \sum_{j=0}^{k} \beta_j(\tau) y(t_{n+j})\right). \tag{2.7}$$

From the traditional theorem characterizing the error of the polynomial interpolation [1], it follows easily that $\mathcal{L}$ and Φ can be expanded as

$$\begin{aligned} \mathcal{L}[y(t_n), h] &= C_{k+1}(\tau) h^{k+1} y^{(k+1)}(t_n) + \mathrm{O}(h^{k+2}), \\ \Phi[y(t_n), h, \tau] &= C_{k+1}(\tau) h^{k+1} y^{(k+1)}(t_n) + \mathrm{O}(h^{k+2}). \end{aligned} \tag{2.8}$$

Therefore, when $C_{k+1}(\tau) \neq 0$, the OLM_k formula (2.1) and the LMM_k formula (2.4) have the same order k and the same error constant $C_{k+1}(\tau)$. When $C_{k+1}(\tau) = 0$, both formulas have order at least $k+1$ but they do not have the same error constant in general.

Figure 2.1 depicts the error constant $C_{k+1}(\tau)$ as a function of the ratio τ for $k = 1, \dots, 6$. It also depicts the ratios τ^+ and τ^* mentioned in the introduction. Observe that $\tau = k$ gives the accuracy at the next interpolation point t_{n+k}. The figure indicates that the magnitude of the error constant increases between τ^+ (point t^+) and k (point t_{n+k}). The error constant is zero at time τ^+, indicating that the method is of order $k+1$ with this choice. In addition, the method is always more accurate at ratio τ^* (point t^*) than at ratio k (point t_{n+k}). Observe also that, for $k = 1$, τ^+ and τ^* are the same ratios. For completeness, we give the following theorem which is fundamental in characterizing τ^+.

THEOREM 2.1 (DALHQUIST, 1983). *If the formula* $\mathrm{OLM}_k(\tau)$ *is of order* $k+1$*, then* τ *is a root of* $w'(\tau)$.

The k roots of $w'(\tau)$ are located in $]0,1[,]1,2[, \dots,]k-1,k[$. For stability reasons, it will become clear (see Figure 2.2 to be presented shortly) that the *rightmost* root of $w'(\tau)$ is the only root of practical interest, since the OLM

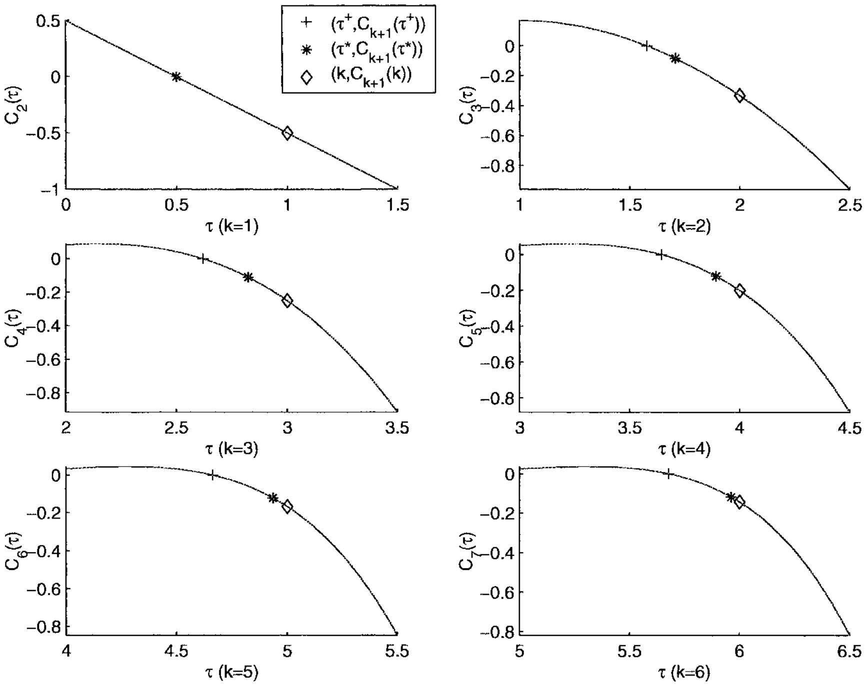

Figure 2.1: The error constant $C_{k+1}(\tau)$ as a function of τ.

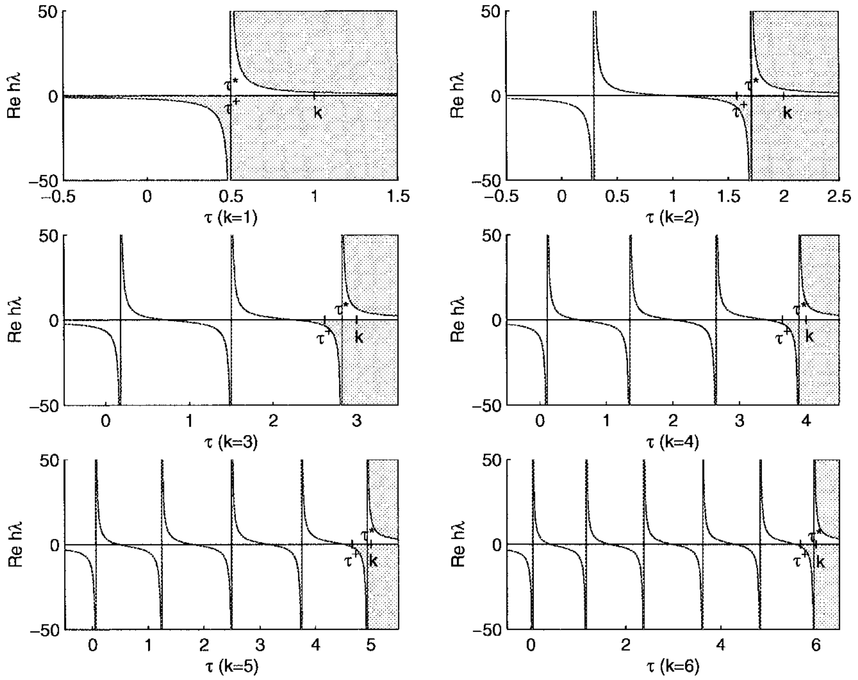

Figure 2.2: The function $\hat{h}(\tau, \pi)$ and stability interval of OLM as a function of τ.

Table 2.1: Values of τ^+ for $1 \le k \le 6$

k	1	2	3	4	5	6
τ^+	0.5	1.5774	2.6180	3.6444	4.6634	5.6781

formula is not zero-stable for the other roots. As a consequence, we define τ^+ as the rightmost root of $w'(\tau)$. Table 2.1 shows the values of τ^+ for various step numbers k ($1 \le k \le 6$).

2.2 Stability.

When the ODE is a linear system $y' = Ay$, the OLM_k formula (2.1) and the LMM_k formula (2.4) become equivalent and the OLM_k formula has the linear stability of (2.4). Consider the first and second characteristic polynomials associated with $\mathrm{OLM}_k(\tau)$:

$$\rho(\tau, x) = \sum_{j=0}^{k} \alpha_j(\tau) x^j ,$$

$$\sigma(\tau, x) = \sum_{j=0}^{k} \beta_j(\tau) x^j .$$

We use the definition of [7] for the stability region which is thus an *open set.* The boundary of the stability region $\mathcal{R}_A$ of $\mathrm{OLM}_k(\tau)$ is (part of) the locus

$$\hat{h}(\tau, \theta) = \rho(\tau, \mathrm{e}^{i\theta}) / \sigma(\tau, \mathrm{e}^{i\theta}), \tag{2.9}$$

where $0 \le \theta \le 2\pi$. Figure 2.2 gives a preview of the stability region of OLM formulas.

In the figure, the curves are the real function $\hat{h}(\tau, \pi)$ and the shaded regions represent the stability interval, i.e., the intersection of $\mathcal{R}_A$ with the real axis, as a function of τ. These shaded regions can be determined by the stability interval of the OLM(k)'s and by using the fact that the stability region of any convergent linear multistep method cannot contain the positive real axis in the neighborhood of the origin (e.g., [7]). Figure 2.2 also indicates the ratios τ^+ and τ^*. Of course, once again, the next interpolation point t_{n+k} is given by $\tau = k$ for an OLM_k formula. The figure shows that the stability interval increases when the evaluation point moves from t_{n+k-1} ($\tau = k - 1$) to t_{n+k} ($\tau = k$). Observe also that the value t^* specified by ratio τ^* is an attractive evaluation point, since its stability interval is precisely $\mathbb{R}_0^-$ (more detailed pictures are given later in the paper). The stability interval at time t^+ also does not intersect $\mathbb{R}^+$ but is significantly smaller than the stability interval for t^*. Points before the last two interpolation points need not be considered, since the corresponding OLM formulas are not zero-stable.

2.3 Linear versus nonlinear formulas.

It is interesting to note that the formula (2.4) requires one more evaluation of the function f than the formula (2.1), because the value $f(t_{n+k}, y_{n+k})$ is needed in the next step to compute y_{n+k+1}. When $C_{k+1}(\tau) \neq 0$, since the formulas (2.1) and (2.4) have same accuracy and stability, (2.1) is to be preferred to (2.4) for computational reasons. However, when $C_{k+1}(\tau) = 0$, the formulas do not have the same accuracy in general. In addition, an error estimate (needed e.g. for variable step size implementation) for (2.1) may be more expensive in this case because its local error does not have a simple structure like (2.4) does. It is thus not clear which of the two formulas should be preferred in this case.

3 Precisely A(α)-stable One-Leg Multistep methods.

This section is the core of the paper and it studies OLM_k formulas of order k. The error constant $C_{k+1}(\tau)$ of these formulas is not zero. Hence, in our analysis, we do not distinguish between the OLM formula (2.1) and its linear form (2.4), since they have the same accuracy and stability. We will show that it is possible to find a ratio τ^* such that the stability region and the accuracy of $\mathrm{OLM}_k(\tau^*)$ improve upon those of BDF_k. We first define the concept of precise A(α)-stability formally. As mentioned in the introduction, it is motivated by Lambert who argues that the ideal stability region for a method is $\mathbb{C}_0^-$ [7]. We will show that OLM_k formulas come close to that ideal.

Definition 3.1 (Precise A(α)-stability). *A method with stability region $\mathcal{R}_A$ is said to be* precisely *A(α)*-stable, $0 < \alpha < \pi/2$, *if it is A(α)-stable and $\mathcal{R}_A \cap \mathbb{C}^+ = \emptyset$; it is said to be* precisely *A(0)*-stable *if it is precisely A(α)-stable for some $\alpha \in]0, \pi/2[$; it is said to be* precisely *A*-stable *if $\mathcal{R}_A = \mathbb{C}_0^-$.*⋆

We now show how to choose a ratio τ^* to achieve precise A(α)-stability. We first give a necessary condition for precise A(0)-stability.

Lemma 3.1. *If (τ, θ) is a zero of $\sigma(\tau, \mathrm{e}^{i\theta})$, then $\theta = \pi$.*

Theorem 3.2 (Necessary condition for precise A(α)-stability in OLM). *If the* OLM(τ) *is precisely* A(0)*-stable, then τ is a root of $\sigma(\tau, -1)$.*

Proof. Precise A(0)-stability requires that the stability region be an unbounded set. This implies that τ be a pole of $\hat{h}(\tau, \theta)$, i.e., a zero of $\sigma(\tau, \mathrm{e}^{i\theta})$ for some θ. By Lemma 3.1, τ must be a root of $\sigma(\tau, \mathrm{e}^{i\pi}) = \sigma(\tau, -1)$. □

Since the roots of $\sigma(\tau, -1)$ are poles of $\hat{h}(\tau, \pi)$, it follows from Figure 2.2 that only the rightmost root is of practical interest since the OLM formulas are not zero-stable for the other roots. As a consequence, we define τ^* as the rightmost root of $\sigma(\tau, -1)$. Table 3.1 shows the values of τ^* for various step numbers k ($1 \leq k \leq 6$). We now study the properties of $\mathrm{OLM}_k(\tau^*)$. The following proposition is easily verified.

⋆ Precise A(0)-stability simply means that there exists an $\alpha \in]0, \pi/2[$ such that the method is precisely A(α)-stable. It is a convenient notation to avoid naming the particular α.

Table 3.1: Values of τ^* for $1 \le k \le 6$

k	1	2	3	4	5	6
τ^*	0.5	1.7071	2.8229	3.8924	4.9350	5.9613

PROPOSITION 3.3. *τ is a root of $\sigma(\tau,-1)$ iff* $\lim_{\substack{\theta\to\pi\\ \theta<\pi}} \operatorname{Im}\hat{h}(\tau,\theta) = +\infty$ *and* $\lim_{\substack{\theta\to\pi\\ \theta>\pi}} \operatorname{Im}\hat{h}(\tau,\theta) = -\infty$.

Recall that a method is convergent iff it is zero-stable and consistent.

PROPERTY 1 (STABILITY PROPERTIES OF OLM). Let τ^* be the rightmost root of $\sigma(\tau,-1)$. Then,

(1) For $1 \le k \le 6$, $\mathrm{OLM}_k(\tau^*)$ is convergent and A(0)-stable:

  (a) $\mathrm{OLM}_1(\tau^*)$ and $\mathrm{OLM}_2(\tau^*)$ are precisely A-stable;
  (b) $\mathrm{OLM}_3(\tau^*)$ and $\mathrm{OLM}_4(\tau^*)$ are precisely A(0)-stable;
  (c) $\mathrm{OLM}_5(\tau^*)$ and $\mathrm{OLM}_6(\tau^*)$ are almost precisely A(0)-stable, i.e., the boundary of the stability region marginally invades $\mathbb{C}_0^+$;

(2) For $k \ge 7$, $\mathrm{OLM}_k(\tau^*)$ is not convergent (i.e., it is consistent but not zero-stable).

It is important to emphasize that neither the AM formulas nor the BDF's are precisely A(0)-stable: the AM formulas are not A(0)-stable while the stability regions of the BDF's contain part of the positive half-plane $\mathbb{C}^+$. As a consequence, the OLM_k formulas have some appealing stability properties. Note also that the linear form of $\mathrm{OLM}_1(\tau^*)$ corresponds to the Trapezoidal Rule. Finally, the formula $\mathrm{OLM}_2(\tau^*)$ shares three common properties with the Trapezoidal Rule: it is precisely A-stable, it is of order 2, and its error constant is $-1/12$.⋆ It can also be verified that the linear form of $\mathrm{OLM}_2(\tau^*)$ formula becomes equivalent to the Trapezoidal Rule when the latter is used as a starting method to compute y_1.

3.1 Comparison to BDF.

We now compare the $\mathrm{OLM}(\tau^*)$'s and BDF's. Table 3.2 compares the error constant and the stability angle of both formulas for various step numbers. The column step ratio percent indicates how much the step size can be increased in $\mathrm{OLM}(\tau^*)$ (in percentage), while still achieving the same accuracy as BDF's. It can be seen that $\mathrm{OLM}(\tau^*)$ formulas are more precise for $2 \le k \le 6$ and that the gain is significant for small step numbers. $\mathrm{OLM}(\tau^*)$ formulas also have a better stability angle in general (except for $k = 3, 4$). Figure 3.1 compares the stability regions of $\mathrm{OLM}(\tau^*)$'s and BDF's for various step numbers. Here we clearly see that $\mathrm{OLM}(\tau^*)$'s are much closer to the ideal stability region

⋆ By the second Dahlquist barrier (e.g., [7]), this is the smallest possible error constant (in magnitude) for a second-order A-stable linear multistep method.

Table 3.2: Accuracy and stability angle of OLM(τ^*) relative to BDF

Order	Error constant			Stability angle		
k	BDF	OLM(τ^*)	Step ratio percent	BDF	OLM(τ^*)	Percent change
2	−1/3	−1/12	59%	90°	90°	0%
3	−0.25	−0.11	23%	86°	84°	−2%
4	−0.2	−0.12	11%	73°	73°	−1%
5	−0.17	−0.12	5%	52°	55°	6%
6	−0.14	−0.12	3%	18°	25°	40%

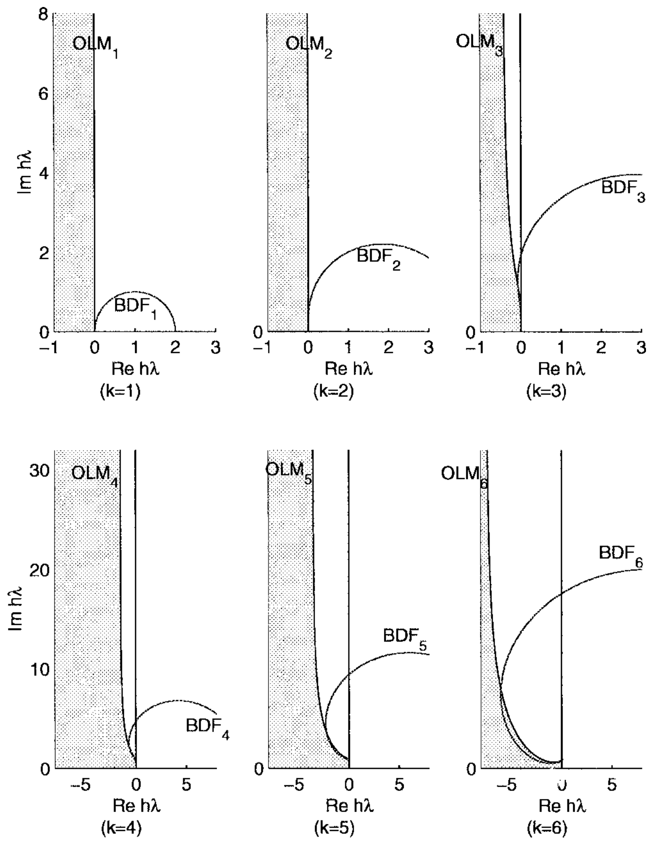

Figure 3.1: Stability regions of OLM(τ^*) and BDF.

than BDF's. OLM(τ^*)'s have almost no intersection with $\mathbb{C}^+$ contrary to BDF's which have significant intersections. Note however that the exact stability regions of the BDF's can be exploited to control the order and the step size of the method [8].

4 Improving the stability of OLM.

In this section, we show how to use the correction idea from Klopfenstein [6] to improve the stability region of OLM formulas. We start by reviewing the basic idea and then we apply it to the OLM's.

4.1 The numerical differentiation formulas.

Klopfenstein [6] introduced a variant of the BDF's, called the numerical differentiation formulas (NDF's), by adding a term to the formula (2.3):

$$\sum_{j=1}^{k} \frac{1}{j} \nabla^j y_{n+k} - hf(t_{n+k}, y_{n+k}) - \kappa\gamma_k \big(y_{n+k} - y_{n+k}^{(0)}\big) = 0, \tag{4.1}$$

where

$$y_{n+k}^{(0)} = \sum_{j=0}^{k} \nabla^j y_{n+k-1} \tag{4.2}$$

is a predictor. In this formula, κ is a parameter and $\gamma_k = \sum_{j=1}^{k} \frac{1}{j}$. By noting that

$$y_{n+k} - y_{n+k}^{(0)} = \nabla^{k+1} y_{n+k} \approx h^{k+1} y^{(k+1)} \tag{4.3}$$

we see that the term added to the formula (2.3) can be interpreted as a correction term which does not decrease the order of the formula. The corresponding error constant is given by

$$-\frac{1}{k+1} - \kappa\gamma_k. \tag{4.4}$$

Shampine and Reichelt [10] proposed values for κ that make the NDF's more accurate than the BDF's while only degrading slightly the stability. Table 4.1 compares the accuracy and the stability angles of the NDF's proposed by Shampine and Reichelt and the traditional BDF's. As can be seen, the correction improves the accuracy, while only decreasing the stability angle slightly.

Table 4.1: Accuracy and stability angle of NDF relative to BDF

Order	Error constant			Stability angle		
k	BDF	NDF	Step ratio percent	BDF	NDF	Percent change
1	−0.5	−0.31	26%	90°	90°	0%
2	−1/3	−1/6	26%	90°	90°	0%
3	−0.25	−0.1	26%	86°	80°	−7%
4	−0.2	−0.11	12%	73°	66°	−10%

4.2 Corrected OLM formulas.

We apply the same corrector idea to the OLM formula (2.1) to obtain:

$$\boxed{p'(t) - f(t, p(t)) - \kappa\gamma_k\big(y_{n+k} - y_{n+k}^{(0)}\big) = 0.} \tag{4.5}$$

The formula (4.5) is denoted OLM$^\kappa$ or, more explicitly, OLM$_k^\kappa$. For any value of κ, the formula OLM$_k^\kappa$ is of order at least k and its error constant is given by

$$C_{k+1}(\tau) - \kappa\gamma_k. \tag{4.6}$$

The boundary of the stability region of OLM$^\kappa(\tau)$ is (part of) the locus

$$\begin{aligned} \hat{h}_\kappa(\tau, \theta) &= \rho_\kappa(\tau, \mathrm{e}^{i\theta})/\sigma_\kappa(\tau, \mathrm{e}^{i\theta}) \\ &= (\mathrm{e}^{i\theta}\rho(\tau, \mathrm{e}^{i\theta}) + \kappa\gamma_k\varrho(\mathrm{e}^{i\theta}))/(\mathrm{e}^{i\theta}\sigma(\tau, \mathrm{e}^{i\theta})) \\ &= \hat{h}(\tau, \theta) + \kappa\gamma_k\varrho(\mathrm{e}^{i\theta})/(\mathrm{e}^{i\theta}\sigma(\tau, \mathrm{e}^{i\theta})), \end{aligned} \tag{4.7}$$

where

$$\varrho(x) = \sum_{j=0}^{k} \varphi_j(k+1)x^j - x^{k+1}. \tag{4.8}$$

The correction preserves the main results about the method.

THEOREM 4.1 (NECESSARY CONDITION FOR PRECISE A(α)-STABILITY IN OLM$^\kappa$). *For all $\kappa \in \mathbb{R}$, if the* OLM$^\kappa(\tau)$ *is precisely* A(0)*-stable, then τ is a root of $\sigma(\tau, -1)$.*

PROOF. By (4.7), precise A(0)-stability implies that τ be a pole of $\hat{h}_\kappa(\tau, \theta)$, i.e., a zero of $\sigma(\tau, \mathrm{e}^{i\theta})$ for some θ. By Lemma 3.1, τ must be a root of $\sigma(\tau, \mathrm{e}^{i\pi}) = \sigma(\tau, -1)$. □

PROPOSITION 4.2. *For all $\kappa \in \mathbb{R}$, τ is a root of $\sigma(\tau, -1)$ iff* $\lim_{\substack{\theta\to\pi \\ \theta<\pi}} \operatorname{Im} \hat{h}_\kappa(\tau, \theta) = +\infty$ *and* $\lim_{\substack{\theta\to\pi \\ \theta>\pi}} \operatorname{Im} \hat{h}_\kappa(\tau, \theta) = -\infty$.

4.3 Determination of the parameters in OLM$^\kappa$.

It remains to determine the value of the parameter κ. Contrary to [10], our objective is to optimize the stability region of the OLM's. We know from Theorem 4.1 and Proposition 4.2 that precise A(0)-stability implies

$$\lim_{\substack{\theta\to\pi \\ \theta<\pi}} \operatorname{Im} \hat{h}_\kappa(\tau, \theta) = +\infty, \qquad \lim_{\substack{\theta\to\pi \\ \theta>\pi}} \operatorname{Im} \hat{h}_\kappa(\tau, \theta) = -\infty. \tag{4.9}$$

To optimize the stability region, we also impose

$$\lim_{\theta\to\pi} \operatorname{Re} \hat{h}_\kappa(\tau, \theta) = 0. \tag{4.10}$$

Table 4.2: Values of κ^* for $1 \le k \le 6$

k	1	2	3	4	5	6
κ^*	0	0	0.0129	0.0213	0.0257	0.0274

This limit L can be computed and is given by

$$\left(\sum_{j=0}^{k} A_j \varphi_j(k+1) - A_{k+1}\right)\kappa\gamma_k + \sum_{j=0}^{k} A_{j+1}\alpha_j(\tau), \tag{4.11}$$

where

$$A_j = B_1 j(-1)^{j+1} + B_2(-1)^j, \quad 0 \le j \le k+1, \tag{4.12}$$

$$B_1 = \left(\sum_{j=0}^{k} \beta_j(\tau)(j+1)(-1)^j\right)^{-1}, \tag{4.13}$$

$$B_2 = -\frac{B_1^2}{2}\sum_{j=0}^{k} \beta_j(\tau)(j+1)^2(-1)^{j+1}. \tag{4.14}$$

As a consequence, there exists a unique value κ^* satisfying condition (4.10) and given by

$$\kappa^* = \frac{\sum_{j=0}^{k} A_{j+1}\alpha_j(\tau)}{\gamma_k\big(A_{k+1} - \sum_{j=0}^{k} A_j\varphi_j(k+1)\big)}. \tag{4.15}$$

Table 4.2 shows the values of κ^* for $1 \le k \le 6$. As for the OLM's, we can verify that only the rightmost root of $\sigma(\tau,-1)$ is of practical interest for $\mathrm{OLM}^{\kappa^*}(\tau)$ since the formula is not zero-stable for the other roots. We now describe the stability properties of the $\mathrm{OLM}^{\kappa^*}(\tau^*)$ formulas.

PROPERTY 2 (STABILITY PROPERTIES OF OLM^{κ^*}). Let τ^* be the rightmost root of $\sigma(\tau,-1)$ and κ^* be defined by (4.15). Then,

(1) For $1 \le k \le 6$, $\mathrm{OLM}_k^{\kappa^*}(\tau^*)$ is convergent and A(0)-stable:
  - (a) $\mathrm{OLM}_1^{\kappa^*}(\tau^*)$ and $\mathrm{OLM}_2^{\kappa^*}(\tau^*)$ are precisely A-stable;
  - (b) $\mathrm{OLM}_3^{\kappa^*}(\tau^*)$ and $\mathrm{OLM}_4^{\kappa^*}(\tau^*)$ are precisely A(0)-stable;
  - (c) $\mathrm{OLM}_5^{\kappa^*}(\tau^*)$ and $\mathrm{OLM}_6^{\kappa^*}(\tau^*)$ are almost precisely A(0)-stable, i.e., the boundary of the stability region marginally invades $\mathbb{C}_0^+$;

(2) $\mathrm{OLM}_7^{\kappa^*}(\tau^*)$ is convergent but not A(0)-stable;

(3) For $k \ge 8$, $\mathrm{OLM}_k^{\kappa^*}(\tau^*)$ is not convergent (i.e., it is consistent but not zero-stable).

4.4 Comparison to BDF/NDF.

It is interesting to compare the corrected OLM formulas with BDF's and NDF's. Table 4.3 compares the accuracy and the stability angles of $\mathrm{OLM}_k^{\kappa^*}(\tau^*)$

Table 4.3: Accuracy and stability angle of $\text{OLM}^{\kappa^*}(\tau^*)$ relative to BDF

Order	Error constant			Stability angle		
k	BDF	$\text{OLM}^{\kappa^*}(\tau^*)$	Step ratio percent	BDF	$\text{OLM}^{\kappa^*}(\tau^*)$	Percent change
3	−0.25	−0.13	17%	86°	86°	0%
4	−0.2	−0.16	4%	73°	77°	5%
5	−0.17	−0.18	−1%	52°	62°	19%
6	−0.14	−0.18	−4%	18°	36°	101%

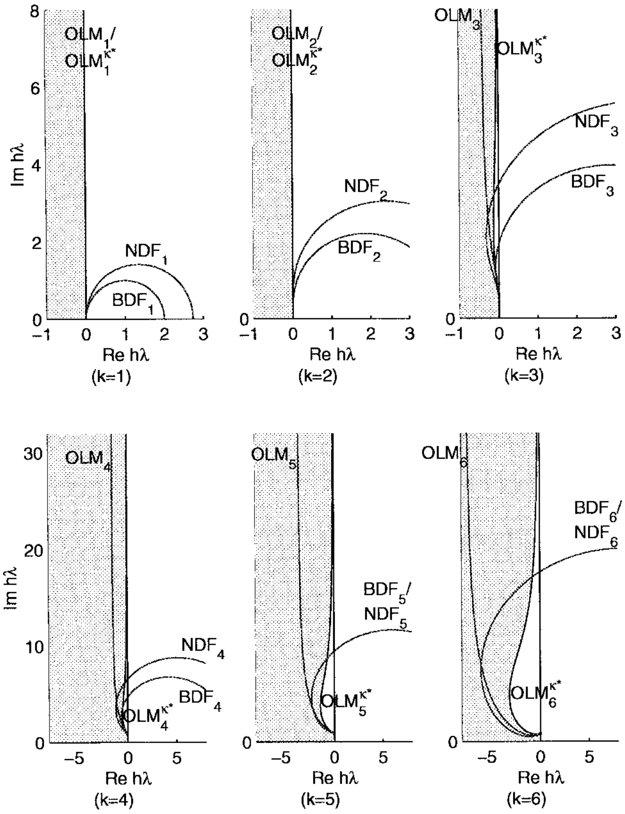

Figure 4.1: Stability regions of $\text{OLM}^{\kappa^*}(\tau^*)$, BDF, and NDF.

for $k = 3..6$. (For $k = 1..2$, $\text{OLM}_k^{\kappa^*}(\tau^*) = \text{OLM}_k(\tau^*)$ since $\kappa^* = 0$.) Observe that $\text{OLM}_k^{\kappa^*}(\tau^*)$ still compares very well to BDF's as far as the error constant is concerned. In addition, $\text{OLM}_k^{\kappa^*}(\tau^*)$ now exhibits significant improvements over BDF's as far as the stability angles are concerned. Figure 4.1 clearly indicates the benefits of the correction on the stability region. For $k = 1..4$, the stability region of $\text{OLM}_k^{\kappa^*}(\tau^*)$ is essentially the ideal stability region. For $k = 5..6$, $\text{OLM}_k^{\kappa^*}(\tau^*)$

also produces a significant improvement over $\mathrm{OLM}_k(\tau^*)$. Clearly, the stability region of $\mathrm{OLM}_k^{\kappa^*}(\tau^*)$ significantly improves over those of BDF's and NDF's.

5 Conclusion

In this paper, we consider one-leg multistep methods for the solution of initial value problems in ODEs. The OLM formulas are derived from the functional equation $p'(t) = f(t, p(t))$, where p is a polynomial approximation of the solution, by carefully choosing an evaluation point t_e. We showed that there exists a point t^* which leads to an OLM formula which is more precise than BDF's, which is (almost) precisely A(α)-stable for a k-step method ($k \leq 6$), and whose stability angle α is essentially similar to BDF's. By applying the corrector idea of Klopfenstein, we showed how to improve the stability region of OLM formulas significantly, while only degrading the accuracy slightly. The resulting formulas are of potential theoretical and practical interest, since precisely A(α)-stable methods were advocated by Lambert [7] from a theoretical standpoint and have found their way into commercial code, since BDF's are not always appropriate in practice.

Finally, it is worth mentioning that the idea of using an evaluation point t that is different from the current integration point t_{n+k} originated from our research on interval methods for parametric differential equations [4]. Although the problem and the issues are quite different as discussed in [5], it is interesting to observe that these nonstandard evaluation points have interesting theoretical and experimental properties in these two contexts.

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