Precisely A(alpha)-stable One-Leg Multistep Method

Micha Janssen and Pascal Van Hentenryck

Department of Computer Science
Brown University
Providence, Rhode Island 02912

CS-02-06
April 2002

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Micha Janssen
UCL
2, Place Sainte Barbe
1348 Louvain-La Neuve
Email: mja@info.ucl.ac.be

Pascal Van Hentenryck
Department of Computer Science
Brown University, Box 1910
Providence, RI 02912
Email: pvh@cs.brown.edu

April 26, 2002

Abstract

We consider One-Leg Multistep (OLM) methods for initial value problems in ODEs. These methods are derived from the functional equation $p'(t) = f(t, p(t))$, where p is a polynomial approximation of the solution. This equation, applied at an evaluation point t_e, produces a nonlinear multistep formula $p'(t_e) = f(t_e, p(t_e))$ which can be used to compute the solution at the next integration point. We show 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 (a concept introduced to capture the ideal stability region) for a k-step method ($k \leq 6$), and whose stability angle α is essentially similar to BDF's. We also show how to apply the corrector idea of Klopfenstein to further improve the stability region.

1 Introduction

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

$$y'(t) = f(t, y(t)) \tag{1}$$

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

$$p'(t) = f(t, p(t)) \tag{2}$$

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 (2), when applied to a specific time t_e, produces an *implicit non-linear multistep* formula

$$p'(t_e) = f(t_e, p(t_e)) \tag{3}$$

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 (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

$$p'(t^+) = f(t^+, p(t^+)) \tag{4}$$

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

$$p'(t^*) = f(t^*, p(t^*)) \tag{5}$$

produces a method with the following properties:

1. It is $A(\alpha)$-stable, its stability angle α is comparable to the one of BDF$_k$, and its stability region does (almost) 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 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], pages 231) concludes his chapter on *Stifness: Linear Stability Thoeory* as follows:

> "Summarizing the two phenomena described above, we can say that methods which are A-stable but not L-stable will, for most problems, produce solutions with slowly damped errors, but these errors can be satisfactorily controlled by an automatic code; L-stable methods do not produce such slowly damped errors but can produce misleading results, which will not be easily detected by an automatic code, when applied to an infrequently met class of problems. On the whole, there seems to be something to be said in favour of what we might call *precisely A-stable* methods, that is, methods whose regions of absolute stability are precisely the left half-plane; the numerical solutions of the test system $y' = Ay$ then tend to zero as n tends to infinity *if and only if* the exact solutions tend to zero as x tends to infinity"

On the other hand, observe that precisely A-stable methods are now finding their way into commercial tools. In particular, Shampine [10] writes

> "The ode15s code of the original MATLAB ODE Suite solves stiff ODEs of the form M(t)y' = f(t,y). It is a variable step size, variable order implementation of a variant of the BDFs called NDFs. For some problems of this form, the damping at infinity of this family of formulas is not appropriate, so a code based on the trapezoidal rule, ode23t, was added to the Suite."

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

$$\boxed{p'(t) - f(t, p(t)) = 0} \tag{6}$$

where

$$\begin{array}{rcl} p(t) & = & \sum_{j=0}^{k} \zeta_j(\tau) \nabla^j y_{n+k}, \\ p'(t) & = & \frac{1}{h} \sum_{j=1}^{k} \zeta_j'(\tau) \nabla^j y_{n+k}, \\ t & = & t_n + \tau h, \\ \zeta_0(\tau) & = & 1, \\ \zeta_j(\tau) & = & \frac{1}{j!} \prod_{m=0}^{j-1} (\tau + m) \;\; (1 \le j \le k), \\ \zeta_j'(\tau) & = & \zeta_j(\tau) \delta_j(\tau) \;\; (1 \le j \le k), \\ \delta_j(\tau) & = & \sum_{m=0}^{j-1} \frac{1}{\tau+m} \;\; (1 \le j \le k). \end{array} \tag{7}$$

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

$$\sum_{j=1}^{k} \frac{1}{j} \nabla^j y_{n+k} - h f(t_{n+k}, y_{n+k}) = 0. \tag{8}$$

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. The following theorem characterizes the error of the polynomial interpolation [1].

Theorem 1 (Error in Polynomial Interpolation) *Let $p(t)$ be the polynomial interpolating the function $y(t)$ at the points $t_0, \ldots, t_k$. Then,*

1. $\exists \xi \in \mathcal{H}\{t_0, \ldots, t_k, t\} : y(t) - p(t) = w(\tau) \frac{y^{(k+1)}(\xi)}{(k+1)!} h^{k+1}$;

2. $\exists \xi_1, \xi_2 \in \mathcal{H}\{t_0, \ldots, t_k, t\} : y'(t) - p'(t) = w'(\tau) \frac{y^{(k+1)}(\xi_1)}{(k+1)!} h^k + w(\tau) \frac{y^{(k+2)}(\xi_2)}{(k+2)!} h^{k+1}$;

where $\mathcal{H}A$ is the hull of set A and the function w is defined as follows

$$w(\tau) = \prod_{j=0}^{k} (\tau - j).$$

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

$$\sum_{j=0}^{k} \alpha_j(\tau) y_{n+j} = h \sum_{j=0}^{k} \beta_j(\tau) f_{n+j} \tag{9}$$

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

$$\begin{array}{rcl} \alpha_j(\tau) & = & \varphi_j'(\tau) \\ \beta_j(\tau) & = & \varphi_j(\tau) \\ \varphi_j(\tau) & = & \prod_{\substack{m=0 \\ m\neq j}}^{k} \frac{\tau+k-m}{j-m} \\ f_{n+j} & = & f(t_{n+j}, y_{n+j}). \end{array} \tag{10}$$

We can easily verify that, for all τ, the formula (9) is normalized, i.e., $\sum_{j=0}^{k} \beta_j(\tau) = 1$. We now show that

1. Formulas (6) and (9) have order at least k;
2. when either formula (6) or (9) has order k, the formulas have the same order and the same error constant (i.e., they have the same accuracy);
3. the formulas (6) and (9) have the same linear stability.

2.1 Accuracy

Consider the linear difference operator

$$\mathcal{L}[y(t_n), h] = \sum_{j=0}^{k} \alpha_j(\tau) y(t_{n+j}) - h \sum_{j=0}^{k} \beta_j(\tau) y'(t_{n+j}) \tag{11}$$

of the linear multistep method (9) and let us associate a difference operator with OLM$_k$

$$\Phi[y(t_n), h, \tau] = \sum_{j=0}^{k} \alpha_j(\tau) y(t_{n+j}) - h f(t, \sum_{j=0}^{k} \beta_j(\tau) y(t_{n+j})). \tag{12}$$

From Theorem 1, it follows easily that $\mathcal{L}$ and Φ can be expanded as

$$\begin{array}{rcl} \mathcal{L}[y(t_n), h] & = & C_{k+1}(\tau) h^{k+1} y^{(k+1)}(t_n) + O(h^{k+2}), \\ \Phi[y(t_n), h, \tau] & = & C_{k+1}(\tau) h^{k+1} y^{(k+1)}(t_n) + O(h^{k+2}). \end{array} \tag{13}$$

Therefore, when $C_{k+1}(\tau) \neq 0$, the OLM$_k$ formula (6) and the LMM$_k$ formula (9) 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 1 depicts the error constant $C_{k+1}(\tau)$ as a function of the ratio τ for $k = 1, \ldots 6$. 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 error constant decreases 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^+.

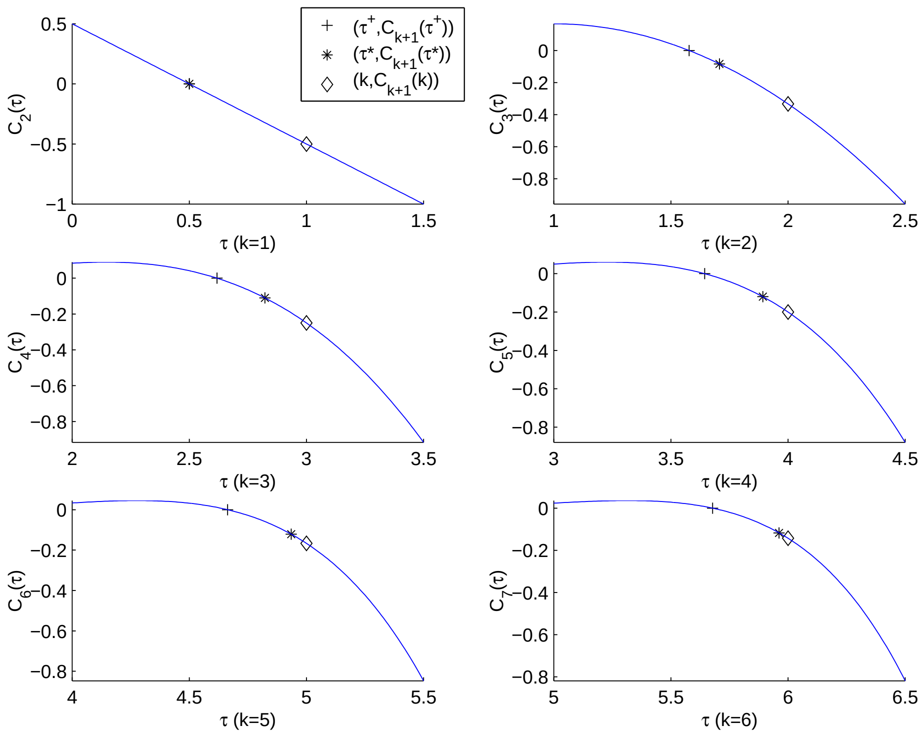

Figure 1: The Error Constant $C_{k+1}(\tau)$ as a Function of τ.

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

Table 1: Values of τ^+ for $1 \leq k \leq 6$.

Theorem 2 (Dalhquist, 1983) *If the formula OLM$_k$(τ) is of order $k+1$, then τ is a root of $w'(\tau)$.*

The k roots of $w'(\tau)$ are located in $]0,1[,]1,2[,\ldots,]k-1,k[$. From For stability reasons, it will be become clear (see Figure 2 to be presented shortly) that the *rightmost* root of $w'(\tau)$ is the only root of practical interest, since the OLM formula is not zero-stable for the other roots. As a consequence, we define τ^+ as the rightmost root of $w'(\tau)$. Table 1 shows the values of τ^+ for various stepnumbers k ($1 \leq k \leq 6$).

2.2 Stability

When the ODE is a linear system $y' = Ay$, the OLM$_k$ formula (6) and the LMM$_k$ formula (9) become equivalent. Therefore, the OLM$_k$ formula has the linear stability of (9).
Consider the first and second characteristic polynomials associated with OLM$_k$(τ):

$$\begin{aligned} \rho(\tau,x) &= \sum_{j=0}^{k} \alpha_j(\tau) x^j \\ \sigma(\tau,x) &= \sum_{j=0}^{k} \beta_j(\tau) x^j . \end{aligned}$$

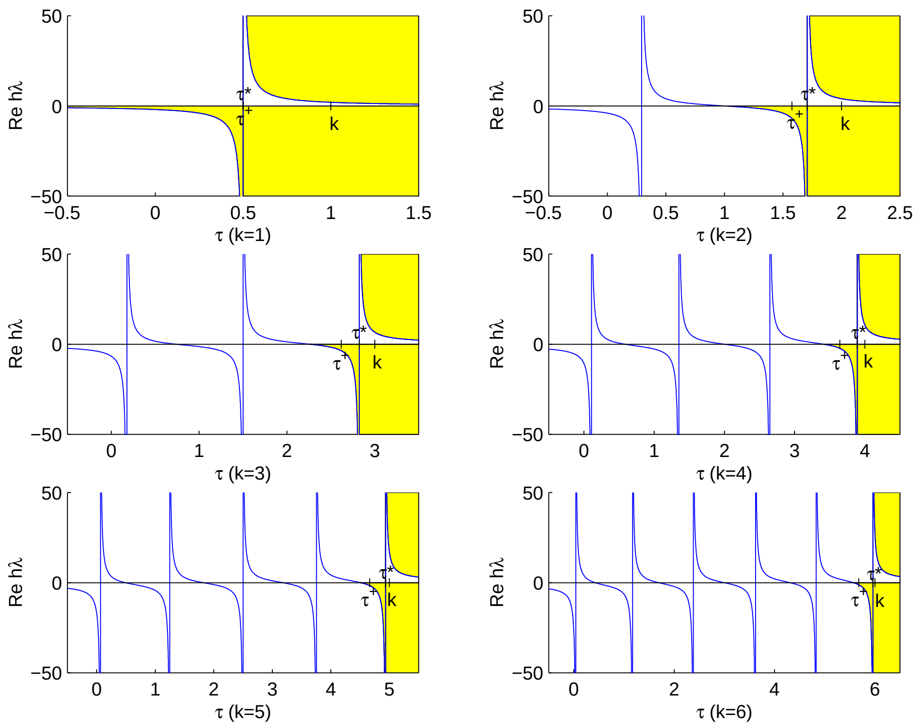

Figure 2: The Function $\hat{h}(\tau, \pi)$ and Stability Interval of OLM as a Function of τ.

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 $\text{OLM}_k(\tau)$ is (part of) the locus

$$\hat{h}(\tau, \theta) = \rho(\tau, e^{i\theta})/\sigma(\tau, e^{i\theta}) \tag{14}$$

where $0 \leq \theta \leq 2\pi$. Figure 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 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 (9) requires one more evaluation of the function f than the formula (6), because the value $f(t_{n+k}, y_{n+k})$ is needed in the next step to compute y_{n+k+1}. When $C_{k+1}(\tau) \neq 0$,

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

Table 2: Values of τ^* for $1 \leq k \leq 6$.

since the formulas (6) and (9) have same accuracy and stability, (6) is to be preferred to (9) 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 for (6) may be more expensive in this case because its local error does not have a simple structure like (9) 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 (6) and its linear form (9), 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 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 ideal stability region for a method is $\mathbb{C}_0^-$ [7]. We will show that OLM$_k$ formulas come close to that ideal.

Definition 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 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 1 *If (τ, θ) is a zero of $\sigma(\tau, e^{i\theta})$, then $\theta = \pi$.*

Theorem 3 (Necessary Condition for Precise A(α)-Stability in OLM) *If the method 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 $\sigma(\tau, e^{i\theta})$ for some θ. By Lemma 1, τ must be a root of $\sigma(\tau, e^{i\pi}) = \sigma(\tau, -1)$. $\Box$

Since the roots of $\sigma(\tau, -1)$ are poles of $\hat{h}(\tau, \pi)$, it follows from Figure 1 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 2 shows the values of τ^* for various stepnumbers k ($1 \leq k \leq 6$). We now study the properties of OLM$_k(\tau^*)$. The following proposition is easily verified.

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

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 $1 \leq k \leq 6$, OLM$_k(\tau^*)$ is convergent and A(0)-stable:*
   (a) *OLM$_1(\tau^*)$ and OLM$_2(\tau^*)$ are precisely A-stable;*

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%

Table 3: Accuracy and stability angle of OLM(τ^*) relative to BDF.

(b) OLM$_3(\tau^*)$ and OLM$_4(\tau^*)$ are precisely A(0)-stable;

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

2. For $k \geq 7$, 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 appealling stability properties. Note also that, for $k = 1$, we have $\tau^* = \tau^+$. Finally, the formula OLM$_2(\tau^*)$ shares three common properties with the Trapezoidal Rule:

1. it is precisely A-stable;
2. it is of order 2;
3. its error constant is -1/12.[1]

It can also be verified that the linear OLM$_2(\tau^*)$ formula becomes equivalent to the Trapezoidal Rule when the latter is used as a starting method to compute the value y_1.

3.1 Comparison to BDF

We now compare the OLM(τ^*)'s and BDF's. Table 3 compares the error constant and the stability angle of both formulas for various stepnumbers. It can be seen that OLM(τ^*) formulas are more precise for $2 \leq k \leq 6$ and that the gain is significant for small stepnumbers. OLM(τ^*) formulas also have a better stability angle in general (except for $k = 3, 4$). Figure 3 is also very interesting. It compares the stability regions of OLM(τ^*)'s and BDF's for various stepnumbers. Here we clearly see that OLM(τ^*)'s are much closer to the ideal stability region than BDF's. OLM(τ^*)'s have almost no intersection with $\mathbb{C}^+$ contrary to BDF's which have significant intersections.

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.

[1] 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.

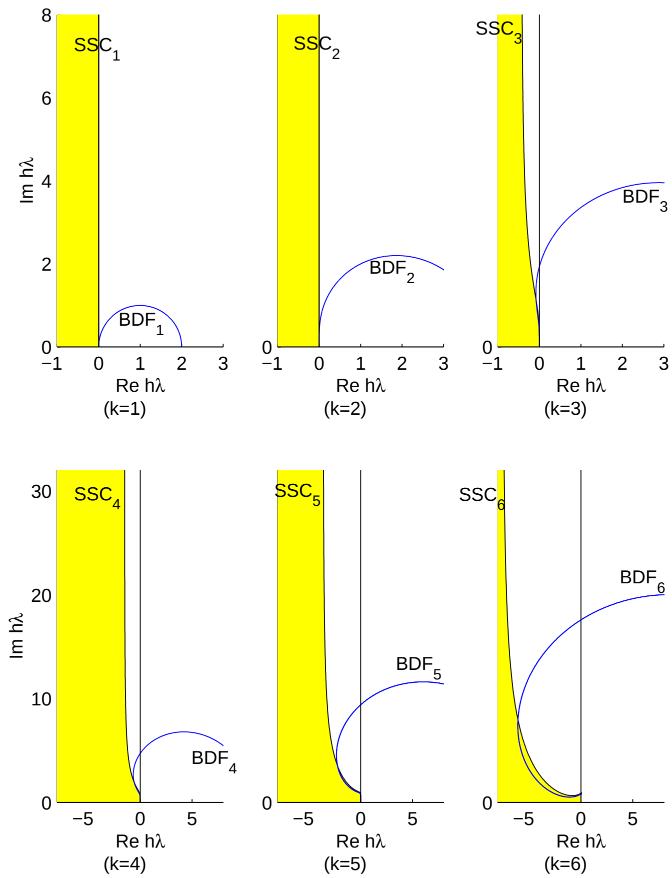

Figure 3: Stability regions of OLM(τ^*) and BDF.

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 (8):

$$\sum_{j=1}^{k} \frac{1}{j} \nabla^j y_{n+k} - hf(t_{n+k}, y_{n+k}) - \kappa\gamma_k \left(y_{n+k} - y_{n+k}^{(0)} \right) = 0 \tag{15}$$

where

$$y_{n+k}^{(0)} = \sum_{j=0}^{k} \nabla^j y_{n+k-1} \tag{16}$$

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

$$y_{n+k} - y_{n+k}^{(0)} = \nabla^{k+1} y_{n+k} \approx h^{k+1} y^{(k+1)} \tag{17}$$

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%

Table 4: Accuracy and stability angle of NDF relative to BDF.

we see that the term added to the formula (8) can be interpreted as a correction term which does not decrease the order of the formula. The corresponding error constant is given by

$$-\frac{1}{k+1} - \kappa\gamma_k. \tag{18}$$

Shampine and Reichelt [9] proposed values for κ that make the NDF's more accurate than the BDF's while only degrading slightly the stability. Table 4 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 (by about 26% in step ratio percentage on orders 1 to 3) while only decreasing the stability angle slightly.

4.2 Corrected OLM Formulas

We apply the same corrector idea to the OLM formula (6) to obtain:

$$\boxed{p'(t) - f(t, p(t)) - \kappa\gamma_k \left(y_{n+k} - y_{n+k}^{(0)}\right) = 0.} \tag{19}$$

The formula (19) 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

$$C_{k+1}(\tau) - \kappa\gamma_k. \tag{20}$$

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

$$\begin{aligned} \hat{h}_\kappa(\tau, \theta) &= \rho_\kappa(\tau, e^{i\theta})/\sigma_\kappa(\tau, e^{i\theta}) \\ &= \left(e^{i\theta}\rho(\tau, e^{i\theta}) + \kappa\gamma_k\varrho(e^{i\theta})\right)/(e^{i\theta}\sigma(\tau, e^{i\theta})) \\ &= \hat{h}(\tau, \theta) + \kappa\gamma_k\varrho(e^{i\theta})/(e^{i\theta}\sigma(\tau, e^{i\theta})) \end{aligned} \tag{21}$$

where

$$\varrho(x) = \sum_{j=0}^{k} \varphi_j(k+1)x^j - x^{k+1}. \tag{22}$$

The correction preserves the main results about the method.

Theorem 4 (Necessary Condition for Precise A(α)-Stability in OLM$^\kappa$) *For all $\kappa \in \mathbb{R}$, if the method OLM$^\kappa(\tau)$ is precisely A(0)-stable, then τ is a root of $\sigma(\tau, -1)$.*

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

Table 5: Values of κ^* for $1 \leq k \leq 6$.

Proof By (21), precise A(0)-stability implies that τ be a pole of $\hat{h}_\kappa(\tau,\theta)$, i.e., a zero of $\sigma(\tau, e^{i\theta})$ for some θ. By Lemma 1, τ must be a root of $\sigma(\tau, e^{i\pi}) = \sigma(\tau, -1)$. □

Proposition 2 *For all* $\kappa \in \mathbb{R}$, τ *is a root of* $\sigma(\tau,-1)$ *iff* $\lim_{\substack{\theta\to\pi \\ \theta<\pi}} \text{Im } \hat{h}_\kappa(\tau,\theta) = +\infty$ *and* $\lim_{\substack{\theta\to\pi \\ \theta>\pi}} \text{Im } \hat{h}_\kappa(\tau,\theta) = -\infty$.

4.3 Determination of the Parameters in OLM$^\kappa$

It remains to determine the value of the parameter κ. Contrary to [9], our objective is to optimize the stability region of the OLM's. We know from Theorem 4 and Proposition 2 that precise A(0)-stability implies

$$\lim_{\substack{\theta\to\pi \\ \theta<\pi}} \text{Im } \hat{h}_\kappa(\tau,\theta) = +\infty, \quad \lim_{\substack{\theta\to\pi \\ \theta>\pi}} \text{Im } \hat{h}_\kappa(\tau,\theta) = -\infty. \tag{23}$$

To optimize the stability region, we also impose

$$L = \lim_{\theta\to\pi} \text{Re } \hat{h}_\kappa(\tau,\theta) = 0. \tag{24}$$

This limit L can be computed and is given by

$$L = \left(\sum_{j=0}^{k} A_j \varphi_j(k+1) - A_{k+1} \right) \kappa\gamma_k + \sum_{j=0}^{k} A_{j+1}\alpha_j(\tau) \tag{25}$$

where

$$A_j = B_1 j(-1)^{j+1} + B_2(-1)^j, \;\; 0 \leq j \leq k+1, \tag{26}$$

$$B_1 = \left(\sum_{j=0}^{k} \beta_j(\tau)(j+1)(-1)^j \right)^{-1}, \tag{27}$$

$$B_2 = -\frac{B_1^2}{2} \sum_{j=0}^{k} \beta_j(\tau)(j+1)^2(-1)^{j+1}. \tag{28}$$

As a consequence, there exists a unique value κ^* satisfying condition (24) and given by

$$\kappa^* = \frac{\sum_{j=0}^{k} A_{j+1}\alpha_j(\tau)}{\gamma_k \left(A_{k+1} - \sum_{j=0}^{k} A_j \varphi_j(k+1) \right)}. \tag{29}$$

Table 5 shows the values of κ^* for $1 \leq k \leq 6$. As for the OLM's, we can verify that only the rightmost root of $\sigma(\tau,-1)$ is of practical interest for OLM$^{\kappa^*}(\tau)$ since the formula is not zero-stable for the other roots. We now describe the stability properties of the OLM$^{\kappa^*}(\tau^*)$ formulas.

Order	Error constant			Stability angle		
k	BDF	$\mathrm{OLM}^{\kappa^*}(\tau^*)$	Step ratio percent	BDF	$\mathrm{OLM}^{\kappa^*}(\tau^*)$	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%

Table 6: Accuracy and stability angle of $\mathrm{OLM}^{\kappa^*}(\tau^*)$ relative to BDF.

Property 2 (Stability Properties of OLM^{κ^*}) *Let τ^* be the rightmost root of $\sigma(\tau, -1)$ and κ^* be defined by (29). Then,*

1. *For $1 \le k \le 6$, $OLM_k^{\kappa^*}(\tau^*)$ is convergent and A(0)-stable:*
   - *(a) $OLM_1^{\kappa^*}(\tau^*)$ and $OLM_2^{\kappa^*}(\tau^*)$ are precisely A-stable;*
   - *(b) $OLM_3^{\kappa^*}(\tau^*)$ and $OLM_4^{\kappa^*}(\tau^*)$ are precisely A(0)-stable;*
   - *(c) $OLM_5^{\kappa^*}(\tau^*)$ and $OLM_6^{\kappa^*}(\tau^*)$ are almost precisely A(0)-stable, i.e., the boundary of the stability region marginally invades $\mathbb{C}_0^+$;*
2. *$OLM_7^{\kappa^*}(\tau^*)$ is convergent but not A(0)-stable;*
3. *For $k \ge 8$, $OLM_k^{\kappa^*}(\tau^*)$ 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 6 compares the accuracy and the stability angles of $\mathrm{OLM}_k^{\kappa^*}(\tau^*)$ for $k = 3..6$. (For $k = 1..2$, $\mathrm{OLM}_k^{\kappa^*}(\tau^*)$ = $\mathrm{OLM}_k(\tau^*)$ since $\kappa^* = 0$.) Observe that $\mathrm{OLM}_k^{\kappa^*}(\tau^*)$ still compares very well to BDF's as far as the error constant is concerned. In addition, $\mathrm{OLM}_k^{\kappa^*}(\tau^*)$ now exhibits significant improvements over BDF's as far as the stability angles are concerned. Figure 4 is also particularly interesting. It clearly indicates the benefits of the correction on the stability region. For $k = 1..4$, the stability region of $\mathrm{OLM}_k^{\kappa^*}(\tau^*)$ is essentially the ideal stability region. For $k = 5..6$, $\mathrm{OLM}_k^{\kappa^*}(\tau^*)$ 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 ($k \le 6$), 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.

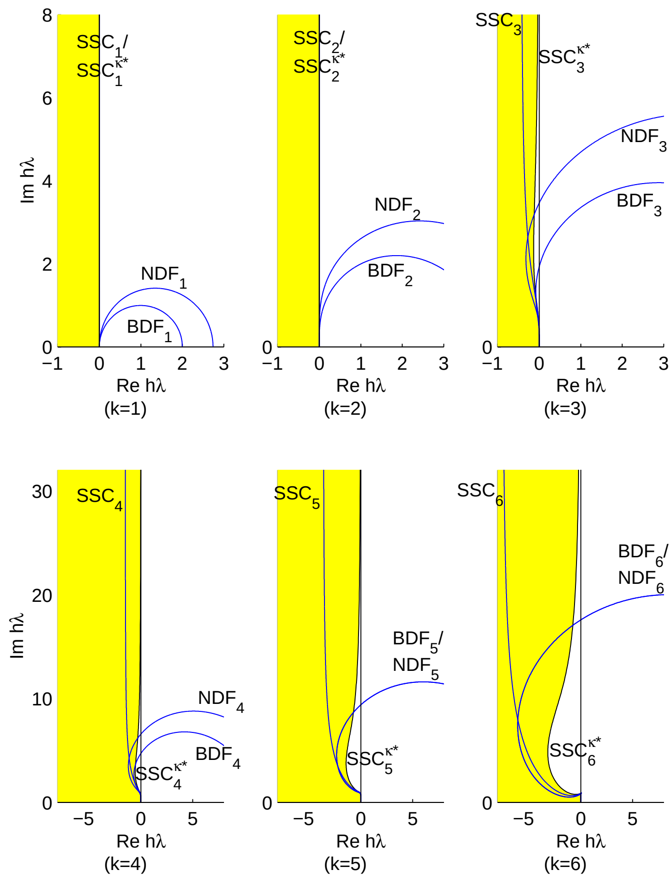

Figure 4: Stability regions of OLM$^{\kappa^*}(\tau^*)$, BDF, and NDF.

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 non-standard evaluation points have interesting theoretical and experimental properties in these two contexts.

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