MAXIMUM ANGLES OF A(ϑ)-STABILITY OF BACKWARD DIFFERENCE FORMULAE

GEORGIOS AKRIVIS AND EMMANOUIL KATSOPRINAKIS

Abstract. We determine the maximum angles ϑ_q for which the three-, four-, five- and six-step backward difference formula (BDF) methods are A(ϑ_q)-stable, slightly improving the well–known angles.

1. Introduction and statement of the result

Let α and β be the generating polynomials of the q-step backward difference formula (BDF) method,

$$\alpha(\zeta)=\sum_{j=1}^{q}\frac{1}{j}\zeta^{q-j}(\zeta-1)^j=\sum_{i=0}^{q}\alpha_i\zeta^i,\quad \beta(\zeta)=\zeta^q, \tag{1}$$

$q=1,\dots,6$. It is well known that the q-step BDF method is A(ϑ_q)-stable with $\vartheta_1=\vartheta_2=90°$, $\vartheta_3\approx 86.03°$, $\vartheta_4\approx 73.35°$, $\vartheta_5\approx 51.84°$, and $\vartheta_6\approx 17.84°$; see [3, Section V.2]. In this note, we give precise expressions of the maximum angles $\vartheta_q, q=3,4,5,6$, slight improvements of the known approximations; see Theorem 1.

Let $h>0$ be an arbitrary constant time step, $t^n:=nh, n\in\mathbb{N}_0$, and $y^0,\dots,y^{q-1}\in\mathbb{C}$ be arbitrary starting approximations to the initial value 1. We consider the discretization of Dahlquist's first test problem, here with flipped sign of the complex constant λ,

$$\begin{cases} y'(t)+\lambda y(t)=0, & t\geqslant 0,\\ y(0)=1, \end{cases}$$

cf. [1] and [6], by the q-step BDF method, i.e., we recursively define approximations $y^n, n\geqslant q$, to the nodal values $y(t^n)$ as follows:

$$\sum_{i=0}^{q}\alpha_i y^{n+i}+h\lambda y^{n+q}=0,\quad n\in\mathbb{N}_0. \tag{2}$$

Since α_q is positive, the approximations $y^n, n\geqslant q$, are well defined by (2) if $\operatorname{Re}\lambda\geqslant 0$.

Let ϑ_q denote the maximum half-angle of the stability sector $S_{\vartheta_q}:=\{z\in\mathbb{C}: z=\rho e^{i\varphi}, \rho>0, |\varphi|<\vartheta_q\}$ of the q-step BDF method, i.e., of the maximal sector contained in the stability region of the method that consists of the points $z=h\lambda\in\mathbb{C}$ such that the solutions of (2) remain bounded.

Our result is:

Date: February 20, 2019.

2010 *Mathematics Subject Classification.* Primary 65L06, 65L20; Secondary 65L04.

Key words and phrases. Test equation, BDF methods, A(ϑ)-stability, maximum angles.

Theorem 1 (Maximum angles of A$(\boldsymbol{\vartheta})$-stability of BDF methods)**.** *The maximum angles ϑ_q for which the q-step BDF methods, $q = 3, 4, 5, 6,$ are A(ϑ_q)-stable are*

$$\begin{cases} \vartheta_3 = \arcsin \dfrac{329\sqrt{7}}{242\sqrt{13}}, & \vartheta_4 = \arcsin \dfrac{699\sqrt{3}}{25\sqrt{2555}}, \\ \vartheta_5 = \arcsin \dfrac{1}{\sqrt{f_5(\tilde{x}_5)}}, & \vartheta_6 = \arcsin \dfrac{45503}{2 \cdot 7^3\sqrt{46879}}, \end{cases}$$

with $\tilde{x}_5 = \frac{223-\sqrt{50825}}{548} \approx -0.004459865605675$ *and*

$$f_5(x) := 1 + \frac{4(1-x)^5(24x^2-3x-11)^2}{(48x^4-150x^3+164x^2-75x+28)^2(1+x)}. \tag{3}$$

We present the proof of Theorem 1 in Section 2.

We note that Nørsett in [4] establishes a criterion for A(ϑ)-stability of multistep methods and applies it to obtain a relation analogous to (5) for high-order BDF methods. He then uses this relation to numerically compute approximations ϑ_q^{N} to the maximum angles. His results, expressed here in degrees rather than in degrees and minutes, the approximations $\vartheta_q^{\mathrm{HW}}$ of [3, Section V.2], as well as the values of ϑ_q, up to a certain precision, are given in Table 1. The discrepancy between ϑ_3^{N} and $\vartheta_3^{\mathrm{HW}}, \vartheta_3$ is due to the fact that, in the notation of [4], the correct polynomial R_3 is twice the one given there.

q	ϑ_q^{N}	$\vartheta_q^{\mathrm{HW}}$	ϑ_q
3	88.45°	86.03°	86.0323668602°
4	73.23333°	73.35°	73.3516704746°
5	51.83333°	51.84°	51.839755836°
6	18.78333°	17.84°	17.8397777922°

TABLE 1. Nørsett's approximations ϑ_q^{N}, the approximations $\vartheta_q^{\mathrm{HW}}$ of [3, Section V.2], and the maximum angles ϑ_q, up to the given precision, for the q-step BDF methods, $q = 3, 4, 5, 6$.

2. Proof of Theorem 1

For $q = 3, 4, 5, 6$, let $d(\zeta) := \alpha(\zeta)/\beta(\zeta)$, for ζ in the unit circle $\mathscr{K}$ in the complex plane, $\mathscr{K} := \{z \in \mathbb{C} : |z| = 1\}$, represent the points of the *root locus curve* of the q-step BDF method. Since β does not have unimodular roots, it is well known that the method is A(ϑ)-stable, for $0 < \vartheta < 90°$, if and only if

$$|\operatorname{Im} d(\zeta)| + (\tan\vartheta) \operatorname{Re} d(\zeta) \geqslant 0 \quad \forall \zeta \in \mathscr{K}, \tag{4}$$

i.e., if and only if the points $-d(\zeta), \zeta \in \mathscr{K}$, lie outside of the sector S_ϑ; see [4, Theorem] and [2, p. 225]. Since (4) is obviously satisfied for nonnegative $\operatorname{Re} d(\zeta)$, we let $\mathscr{K}^-$ be the part of $\mathscr{K}$ given by $\mathscr{K}^- := \{\zeta \in \mathscr{K} : \operatorname{Re} d(\zeta) < 0\}$ and rewrite (4) in the form

$$\frac{1}{\sin\vartheta} \geqslant \sup_{\zeta\in\mathscr{K}^-} \frac{|d(\zeta)|}{|\operatorname{Im} d(\zeta)|}.$$

We infer that

$$\frac{1}{\sin\vartheta_q} = \sup_{\zeta\in\mathscr{K}^-} \frac{|d(\zeta)|}{|\operatorname{Im} d(\zeta)|} =: c_q. \tag{5}$$

The determination of ϑ_q amounts to calculating c_q; then, the maximum angles are $\vartheta_q = \arcsin(1/c_q)$.

From (1) we obtain

$$d(\zeta) = \sum_{i=0}^{q} \alpha_i \zeta^{i-q},$$

and thus, for $\zeta \in \mathscr{K}, \zeta = \mathrm{e}^{\mathrm{i}t} = \cos t + \mathrm{i}\sin t$,

$$d(\zeta) = \sum_{i=0}^{q} \alpha_i \bar{\zeta}^{q-i} = \sum_{\ell=0}^{q} \alpha_{q-\ell}\bar{\zeta}^{\ell} = \sum_{\ell=0}^{q} \alpha_{q-\ell}\mathrm{e}^{-\mathrm{i}\ell t},$$

i.e.,

$$d(\zeta) = \sum_{\ell=0}^{q} \alpha_{q-\ell}\cos(\ell t) - \mathrm{i}\sum_{\ell=1}^{q} \alpha_{q-\ell}\sin(\ell t). \tag{6}$$

Following [4], with $x := \cos t$, we insert in (6) the Chebyshev polynomials T_ℓ and U_ℓ, of the first and the second kind, respectively, $\cos(\ell t) = T_\ell(x)$ and $\sin(\ell t) = \sin t\, U_{\ell-1}(x)$, see, for instance, [5, (1.2) and (1.23)], and obtain

$$d(\zeta) = \sum_{\ell=0}^{q} \alpha_{q-\ell}T_\ell(x) - \mathrm{i}\sin t\sum_{\ell=1}^{q} \alpha_{q-\ell}U_{\ell-1}(x). \tag{7}$$

Furthermore, since $d(\bar{\zeta}) = \overline{d(\zeta)}$ —the root locus curve is symmetric with respect to the real axis— it suffices to take the supremum over all $\zeta \in \mathscr{K}^-$ with nonnegative imaginary part in (5); then, $\sin t \geqslant 0$, and (7) can be rewritten in the form

$$d(\zeta) = \sum_{\ell=0}^{q} \alpha_{q-\ell}T_\ell(x) - \mathrm{i}\sqrt{1-x^2}\sum_{\ell=1}^{q} \alpha_{q-\ell}U_{\ell-1}(x). \tag{8}$$

Let

$$p_q(x) := -\sum_{\ell=1}^{q} \alpha_{q-\ell}U_{\ell-1}(x), \quad r_q(x) := \sum_{\ell=0}^{q} \alpha_{q-\ell}T_\ell(x), \quad x \in [-1,1]. \tag{9}$$

Then, we have

$$p_3(x) = \frac{1}{3}(4x^2 - 9x + 8), \qquad r_3(x) = \frac{1}{3}(1-x)^2(1-4x),$$

$$p_4(x) = \frac{1}{3}(8 - 15x + 16x^2 - 6x^3), \qquad r_4(x) = \frac{2}{3}(x-1)^3(3x+1),$$

$$p_5(x) = \frac{1}{15}(48x^4 - 150x^3 + 164x^2 - 75x + 28), \quad r_5(x) = \frac{2}{15}(1-x)^3(24x^2 - 3x - 11),$$

and

$$p_6(x) = \frac{1}{15}(8-15x+184x^2-370x^3+288x^4-80x^5), r_6(x) = \frac{2}{15}(1-x)^4(40x^2+16x-11).$$

For each q, we have $\zeta \in \mathscr{K}^-$, i.e., $\operatorname{Re} d(\zeta) < 0$, if and only if $r_q(x) < 0$. It is easily seen that, for $x \in [-1,1]$, we have $r_q(x) < 0$ if and only if $x \in I_q := (x_{q,1}, x_{q,2})$, with $x_{3,1} = 1/4, x_{3,2} = 1, x_{4,1} = -1/3, x_{4,2} = 1$, and

$$x_{5,1} = \frac{3-\sqrt{1065}}{48},\ x_{5,2} = \frac{3+\sqrt{1065}}{48}, \quad x_{6,1} = \frac{-4-3\sqrt{14}}{20},\ x_{6,2} = \frac{-4+3\sqrt{14}}{20}.$$

With the notation introduced above, let

$$f_q(x) := 1 + \frac{[r_q(x)]^2}{(1-x^2)[p_q(x)]^2} = 1 + \frac{|\operatorname{Re} d(\zeta)|^2}{|\operatorname{Im} d(\zeta)|^2} = \frac{|d(\zeta)|^2}{|\operatorname{Im} d(\zeta)|^2} \quad \text{for} \quad x \in I_q;$$

cf. (8) and (9), and the definition of c_q in (5). Notice that this definition is compatible with (3) for $q = 5$. It is easily seen that

$$(c_q)^2 = \sup_{x \in I_q} f_q(x); \tag{10}$$

we determine these suprema for each case separately.

Since $r_q(1) = r_q'(1) = 0$, the second rational function on the right-hand side of the following expression for the derivative f_q' of f_q,

$$f_q'(x) = \frac{2r_q(x)}{(1+x)^2[p_q(x)]^3} \frac{[(1-x^2)r_q'(x) + xr_q(x)]p_q(x) - (1-x^2)r_q(x)p_q'(x)}{(1-x)^2},$$

is a polynomial. More precisely, we have

$$\begin{aligned}
f_3'(x) &= \frac{2}{9}\frac{(1-x)^2(1-4x)(22x-13)}{(1+x)^2[p_3(x)]^3}, && \frac{1}{4} < x < 1,\\
f_4'(x) &= \frac{40}{9}\frac{(1-x)^4(3x+1)(1-5x)}{(1+x)^2[p_4(x)]^3}, && -\frac{1}{3} < x < 1,\\
f_5'(x) &= -\frac{8}{225}(1-x)^4\frac{(24x^2-3x-11)(274x^2-223x-1)}{(1+x)^2[p_5(x)]^3}, && x_{5,1} < x < x_{5,2},\\
f_6'(x) &= -\frac{56}{75}(1-x)^6\frac{(40x^2+16x-11)(28x^2-12x-1)}{(1+x)^2[p_6(x)]^3}, && x_{6,1} < x < x_{6,2}.
\end{aligned}$$

The denominators of f_q' are positive since the polynomials $p_3, \dots, p_6$ are positive in the interval $[-1,1]$. This is obvious for p_3, since it does not have real roots. Writing $3p_4$ in the form $3p_4(x) = (1-x)(6x^2-10x+5)+3$, we see that $p_4(x) > 0$ for $-1 \leqslant x \leqslant 1$. Similarly, we write $15p_5$ in the form $15p_5(x) = 12(2x^2-3x+1)^2+(1-x)(6x^2-2x+1)+15$ and see that it is also positive in $[-1,1]$. Finally, $15p_6(x) = x^2(3-2x)(40x^2-84x+59)+(x-1)(7x-8)$; since $40x^2-84x+59$ is positive for all real x, we infer that p_6 is positive in the interval $[-1,1]$.

Three-step method: The derivative of f_3 is positive in the interval $(1/4, 13/22)$ and negative in $(13/22, 1)$, whence f_3 is increasing in $(1/4, 13/22)$ and decreasing in

$(13/22, 1)$. Thus, it attains its maximum in the interval $(1/4, 1)$ at $\tilde{x}_3 := 13/22$. In view of (10), we have

$$(c_3)^2 = \sup_{\frac{1}{4}<x<1} f_3(x) = f_3\Big(\frac{13}{22}\Big) = \frac{242^2 \cdot 13}{329^2 \cdot 7},$$

whence

$$c_3 = \frac{242\sqrt{13}}{329\sqrt{7}} \approx 1.002402460889713.$$

In view of (5), this relation yields the desired expression for ϑ_3.

Four-step method: The derivative of f_4 is positive in $(-1/3, 1/5)$ and negative in $(1/5, 1)$. Thus, f_4 attains its maximum in $(-1/3, 1)$ at $\tilde{x}_4 := 1/5$; now,

$$f_4\Big(\frac{1}{5}\Big) = \frac{25^2 \cdot 2555}{699^2 \cdot 3},$$

whence (10) yields

$$c_4 = \frac{25\sqrt{2555}}{699\sqrt{3}} \approx 1.043752810234182.$$

In view of (5), this relation yields the desired result for ϑ_4.

Five-step method: The roots of the quadratic polynomial $274x^2 - 223x - 1$ are

$$x_{5,3} := \frac{223 - \sqrt{50825}}{548} \quad \text{and} \quad x_{5,4} := \frac{223 + \sqrt{50825}}{548};$$

notice that $-1 < x_{5,1} < x_{5,3} < 0 < x_{5,2} < x_{5,4} < 1$. We easily see that f_5' is positive in the interval $(x_{5,1}, x_{5,3})$ and negative in $(x_{5,3}, x_{5,2})$, whence f_5 attains its maximum in the interval $(x_{5,1}, x_{5,2})$ at $\tilde{x}_5 = x_{5,3} = \frac{223-\sqrt{50825}}{548}$. Therefore, (10) yields

$$c_5 = \sqrt{f_5(\tilde{x}_5)} \approx 1.271802188327223.$$

In view of (5), this relation yields the desired result for ϑ_5.

Six-step method: The roots of the quadratic polynomial $28x^2 - 12x - 1$ are

$$x_{6,3} := -\frac{1}{14} \quad \text{and} \quad x_{6,4} := \frac{1}{2};$$

we have $-1 < x_{6,1} < x_{6,3} < 0 < x_{6,2} < x_{6,4} < 1$. We easily see that f_6' is positive in the interval $(x_{6,1}, x_{6,3})$ and negative in $(x_{6,3}, x_{6,2})$. We infer that f_6 attains its maximum in the interval $I_6 = (x_{6,1}, x_{6,2})$ at $\tilde{x}_6 := x_{6,3} = -\frac{1}{14}$. Therefore, in view of (10),

$$c_6 = \sqrt{f_6\Big(-\frac{1}{14}\Big)} = \frac{\sqrt{45503^2 + 117 \cdot 15^7}}{45503} = \frac{\sqrt{4 \cdot 7^7 \cdot 6697}}{45503} \approx 3.264173650317614.$$

In view of (5), this relation yields the desired result for ϑ_6.

Acknowledgment. The authors would like to thank the anonymous referees; their suggestions led to an improved presentation of the paper.

References

1. G. G. Dahlquist, *A special stability problem for linear multistep methods*, BIT **3**, 27–43 (1963).
2. R. D. Grigorieff, *Numerik gewöhnlicher Differentialgleichungen, Bd.* 2*, Mehrschrittverfahren*, Teubner Studienbücher, Stuttgart (1977).
3. E. Hairer and G. Wanner, *Solving Ordinary Differential Equations II*: *Stiff and Differential–Algebraic Problems*, 2nd revised ed., Springer–Verlag, Berlin Heidelberg, Springer Series in Computational Mathematics v. 14 (2010).
4. S. P. Nørsett, *A criterion for $A(\alpha)$-stability of linear multistep methods*, BIT **9**, 259–263 (1969).
5. T. J. Rivlin, *Chebyshev polynomials. From approximation theory to algebra and number theory*, 2nd ed., Pure and Applied Mathematics. Wiley, New York (1990).
6. O. B. Widlund, *A note on unconditionally stable linear multistep methods*, BIT **7**, 65–70 (1967).

Department of Computer Science & Engineering, University of Ioannina, 451 10 Ioannina, Greece, and Institute of Applied and Computational Mathematics, FORTH, 700 13 Heraklion, Crete, Greece

Email address: akrivis@cse.uoi.gr

Department of Mathematics & Applied Mathematics, University of Crete, 710 03 Heraklion, Crete, Greece

Email address: katsopr@uoc.gr