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Exact BDF stability angles with maple

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Abstract

BDF formulas are among the most efficient methods for numerical integration, in particular of stiff equations (see e.g. Gear in Numerical initial value problems in ordinary differential equations, Prentice Hall, Upper Saddle River, 1971). Their excellent stability properties are known for precisely half a century, from the first calculation of their angles of $A(\alpha)$ -stability by Nørsett (BIT, 9:259–263, 1969). Later, more insight was gained and more precise values were calculated numerically (see for example Hairer and Wanner in Solving ordinary differential equations, Springer, New York, 1996, Sect. V.2). This was the state-of-the-art, when Akrivis and Katsoprinakis (BIT, 2019, <https://doi.org/10.1007/s10543-019-00768-1>) discovered *exact* values for these angles. In this note we simplify the derivation and results by using Maple.

Keywords Stiff differential equations · $A(\alpha)$ -stability · BDF methods

Mathematics Subject Classification 65L07

Let $z = x + iy = e^{i\varphi}$ lie on the unit circle, then the *root locus curve* for k -step BDF is

$$w = u + iv = \sum_{j=1}^k \frac{1}{j} (1 - z^{-1})^j, \quad (0 \leq \varphi \leq 2\pi)$$

(Dedicated to the 75th anniversary of Syvert P. Nørsett.)

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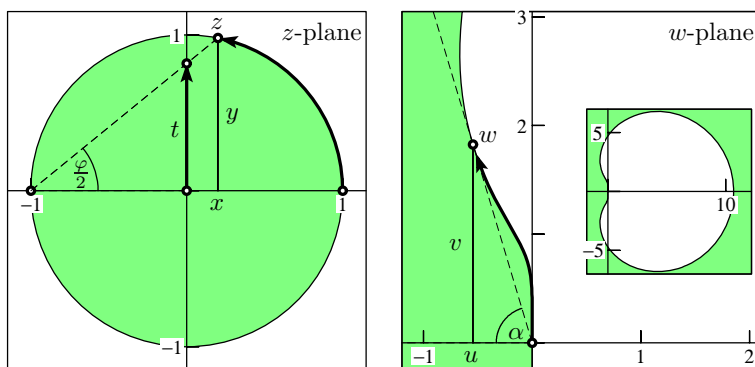


Fig. 1 Root locus curve and stability domain for BDF4

(see e.g., [3, Sect. V.1, Eq. (1.17)]). It describes the boundary of the stability domain (see Fig. 1).

We use the classical parametrization of the unit circle

$$x = \frac{1-t^2}{1+t^2}, \quad y = \frac{2t}{1+t^2}, \quad t = \tan \frac{\varphi}{2}, \quad (-\infty < t < +\infty)$$

(see e.g., Euler's *Calculus Integralis*, Caput V, § 261, 1768). The angle α of $A(\alpha)$ -stability is then computed by the following Maple commands:

```

k:=3; # possible values 3,4,5,6
x:=(1-t^2)/(1+t^2); y:=2*t/(1+t^2); # circle parametrization
w:=simplify(sum(1/j*(1-x+I*y)^j,j=1..k)); # root locus curve w
u:=simplify(evalc(Re(w))); # real part of w
v:=simplify(evalc(Im(w))); # imaginary part of w
p:=simplify(v/(-u)); # tangent of alpha
pd:=simplify(diff(p,t)); # derivative of p
pdn:=factor(numer(pdn)); # factor the numerator
t0:=solve(op(2,pdn),t); # find zeros
p0:=subs(t=t0[1],p); # for k=5 need t0[3]
alpha:=evalf(arctan(p0)/Pi*180); # evaluate angle

```

Here, $p = \tan \alpha = -\frac{v}{u}$, and pdn is the numerator of $\frac{dp}{dt}$, a polynomial in t^2 due to symmetry, whose largest root t_0^2 we have to compute (corresponding to the extremal value w_0 furthest away from the origin). For $k = 3, 4$ and 6 , this t_0^2 is rational, which leads to expressions for $p_0 = \tan \alpha$ containing only one square root (with `Digits:=30`):

k	t_0^2	$p_0 = \tan \alpha$	α
3	$\frac{9}{35}$	$\frac{329}{135}\sqrt{35}$	$86.032366860211647332387423479^\circ$
4	$\frac{2}{3}$	$\frac{699}{512}\sqrt{6}$	$73.351670474578482110409536864^\circ$
5	∞	∞	$51.839755836049910391602721533^\circ$
6	$\frac{15}{13}$	$\frac{45503}{1974375}\sqrt{195}$	$17.839777792245700101632480553^\circ$

The case $k = 5$ is more complicated, since here¹

$$pdn = 15(248t^4 - 275t^2 + 25)(t^2 + 1)^4, \text{ largest root: } t_0^2 = \frac{275}{496} + \frac{5}{496}\sqrt{2033}.$$

Therefore we have to simplify the expression for p_0 by using the field structure of the set $\{a + b\sqrt{2033}; a, b \text{ rationals}\}$. The command `evala(simplify(p0))` in Maple leads to

$$p_0 = \left(-\frac{51844971}{14086400} + \frac{5765167}{70432000}\sqrt{2033} \right) \sqrt{8525 + 155\sqrt{2033}}.$$

Remark By differentiating x (instead of p), we obtain exact values for the values of D in Gear's definition of *stiff stability* (see [2] or [3, p. 250]) as

k	3	4	5	6
D	$\frac{1}{12}$	$\frac{2}{3}$	$\frac{93}{80} + \frac{25}{48}\sqrt{5}$	$\frac{243}{40}$

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¹ The factor $(t^2 + 1)^4$ is related to the order of the method; a similar factor appears for all k and is the deeper reason why the computation of t_0 is so easy.