Step-size coefficients for boundedness of linear multistep methods

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Context

- Presentation is based on the paper L. L., *Exact optimal values of step-size coefficients for boundedness of linear multistep methods*, Numerical Algorithms, 75 (2017)
- Numerical experiments and symbolic proofs have been carried out by using the Wolfram Language (*Mathematica*)
- Consider an initial-value problem u'(t) = F(u(t)) for $t \ge 0$ with $u(0) = u_0$
- Approximate its solution by a linear multistep method (LMM): $u_n = \sum_{j=1}^k a_j u_{n-j} + \Delta t \sum_{j=0}^k b_j F(u_{n-j})$ (for $n \ge k$)
- Basic assumptions on the LMM: consistency, zero-stability, irreducibility, $b_0 \ge 0$
- Monotonicity or boundedness properties play an important role: $\exists ? \mu \ge 1$ such that $||u_n|| \le \mu \max_{0 \le j \le k-1} ||u_j||$ (for $n \ge k$)
- How to guarantee the monotonicity or boundedness property?
- One possibility: impose some restrictions on the step size Δt

Restriction on the step size: SCB or SSP coefficients

Definition 1.2. Suppose that some method coefficients $a_j \in \mathbb{R}$ $(1 \le j \le k)$ and $b_j \in \mathbb{R}$ $(0 \le j \le k)$ satisfying (5) are given. We say that $\gamma > 0$ is a step-size coefficient for boundedness (SCB) of the corresponding LMM, if $\exists \mu \ge 1$ such that

- for any vector space with seminorm $(\mathbb{V}, \|\cdot\|)$,
- for any function $F : \mathbb{V} \to \mathbb{V}$ satisfying

 $\exists \tau > 0 \ \forall v \in \mathbb{V} : \|v + \tau F(v)\| \le \|v\|,$

- for any $\Delta t \in (0, \gamma \tau]$,
- and for any starting vectors $u_j \in \mathbb{V}$ $(0 \le j \le k-1)$,

the sequence u_n generated by (3) has the property $||u_n|| \le \mu \cdot \max_{0 \le j \le k-1} ||u_j||$ for all $n \ge k$.

- If $\mu = 1$, the method is SSP (strong-stability preserving), and $\gamma > 0$ is the SSP coefficient.
- Clearly: larger $\gamma > 0 \implies$ larger step sizes \implies more efficient numerical method

Fundamental questions

- Decide if $\exists \gamma > 0$ SCB or SSP coefficient
- Decide if a given $\gamma > 0$ is an SCB or SSP coefficient
- Find the maximum $\gamma > 0$ SCB or SSP coefficient
- Clearly: $\exists \gamma > 0$ SSP coefficient $\Longrightarrow \gamma$ is an SCB as well
- ◆ It is easy to answer the above questions for SSP coefficients

Existence and computation of SSP coefficients

- There are *simple* (necessary and sufficient) conditions to check whether \exists an SSP coefficient or to find the largest SSP coefficient for a given LMM:
- \exists SSP coefficient \iff

 $b_0 \ge 0,$ $a_j \ge 0,$ $b_j \ge 0$ (for $1 \le j \le k$), and $a_i > 0$ for all $i \in \{1, 2, \dots, k\}$ with $b_i > 0$.

• For a given $\gamma > 0$ to be an SSP coefficient, it is necessary and sufficient:

 $b_0 \ge 0$, and $a_j \ge 0$, $b_j \ge 0$, $\gamma b_j \le a_j$ (for $1 \le j \le k$).

However, for many practically relevant methods: ∄ positive SSP coefficient, but ∃ positive SCB

Existence and computation of SCB

- It is more difficult to check whether \exists an SCB,
- or to determine if a given positive number is a SCB,
- or to compute the maximum SCB–even for a single LMM.
- In W. Hundsdorfer (1954–2017), A. Mozartova, M. N. Spijker, Stepsize restrictions for boundedness and monotonicity of multistep methods, J. Sci. Comput. 50 (2012), 265–286, they define

$$\mu_n(\gamma) := \begin{cases} 0 & \text{for } n < 0, \\ b_n - \gamma \, b_0 \mu_n(\gamma) + \sum_{j=1}^k (a_j - \gamma \, b_j) \mu_{n-j}(\gamma) & \text{for } 0 \le n \le k, \\ - \gamma \, b_0 \mu_n(\gamma) + \sum_{j=1}^k (a_j - \gamma \, b_j) \mu_{n-j}(\gamma) & \text{for } n > k. \end{cases}$$

• Notice that $\mu_n(\gamma)$ is determined *only by the coefficients* of the LMM

Determining if a given positive number is a SCB

• W. Hundsdorfer, A. Mozartova, M. N. Spijker:

Theorem 1.6 Suppose the LMM satisfies (5) and let $\gamma > 0$ be given. Then γ is a SCB if and only if

$$-\gamma \in \operatorname{int}(\mathcal{S}), \text{ and } \mu_n(\gamma) \ge 0 \text{ for all } n \in \mathbb{N}^+.$$
 (8)

- We need to check ∞ many sign conditions
- They typically checked these conditions for $1 \le n \le 1000$ -if \exists positive SCB
- ◆ But what if ∄ positive SCB?

Deciding whether \exists positive SCB

• M. N. Spijker, *The existence of stepsize-coefficients for boundedness of linear multistep methods*, Appl. Numer. Math. 63 (2013) 45–57:

$$\tau_n = \begin{cases} 0 & \text{for } n < 0, \\ b_n + \sum_{j=1}^k a_j \tau_{n-j} & \text{for } 0 \le n \le k, \\ \sum_{j=1}^k a_j \tau_{n-j} & \text{for } n > k. \end{cases}$$

- An *almost* necessary and sufficient condition for \exists positive SCB: the strict positivity of τ_n
- The above sequence is easier to study: no dependence on a parameter (γ)
- The author analyzes the LMM families: Adams–Moulton (or implicit Adams), Adams– Bashforth (or explicit Adams), BDF, extrapolated BDF (EBDF), Milne–Simpson, Nyström

Example (M. N. Spijker)

• Abbreviation here: SCM = step-size coefficient for monotonicity = SSP coefficient

Corollary 2.2 In the EBDF family

- \exists SCM > 0 for the 1-step EBDF method;
- \nexists SCM > 0 but \exists SCB > 0 for the k-step EBDF method with $k \in \{2, 3, 4, 5\}$;
- \nexists SCB > 0 for the 6-step EBDF method.

Exact optimal value γ_{sup} of SCB in the Adams–Bashforth family

- We effectively use the criterion with the parametric sequence: $\mu_n(\gamma) \ge 0$ for all $n \in \mathbb{N}^+$
- In the AB family, $\mu_n(\gamma)$ is a polynomial in γ for each n

Theorem 2.4 *The optimal values of the step-size coefficients for boundedness in the Adams–Bashforth family are given by the rational numbers below:*

- $\gamma_{\sup,1} = 1;$
- $\gamma_{\sup,2} = 4/9 \approx 0.44444;$
- $\gamma_{\text{sup},3} = 84/529 \approx 0.15879;$
- $for k = 4, \nexists SCB > 0.$

Exact optimal values γ_{sup} of SCB in the BDF family for k = 1 and k = 2:

- We again use the criterion with the parametric sequence: $\mu_n(\gamma) \ge 0$ for all $n \in \mathbb{N}^+$
- In the BDF family, $\mu_n(\gamma)$ is a rational function in γ for each n, and it turns out that
 - $\gamma_{\sup,1} = +\infty;$
 - $\gamma_{\sup,2} = 1/2;$
- For k = 1 (implicit Euler method), the corresponding recursion is

 $(\gamma + 1)\mu_n(\gamma) - \mu_{n-1}(\gamma) = 0$ $(n \ge 1)$ with $\mu_0(\gamma) = \frac{1}{\gamma + 1}.$ The explicit solution is $\mu_n(\gamma) = 1/(\gamma + 1)^{n+1} > 0$, so, due to Theorem 1.6, we have that γ is a SCB for any $\gamma > 0$.

• For k = 2, the corresponding recursion is

$$(2\gamma + 3)\mu_n(\gamma) - 4\mu_{n-1}(\gamma) + \mu_{n-2}(\gamma) = 0 \qquad (n \ge 2)$$

with

$$\mu_0(\gamma) = \frac{2}{2\gamma + 3}, \quad \mu_1(\gamma) = \frac{8}{(2\gamma + 3)^2}.$$

Its characteristic polynomial $\mathcal{P}_2(\cdot, \gamma)$ is quadratic for $\gamma > 0$. This polynomial has

- two distinct real roots for $0 < \gamma < 1/2$;
- a double real root for $\gamma = 1/2$;

• a pair of complex conjugate roots for $\gamma > 1/2$.

For any fixed $\gamma > 1/2$ we thus have

$$\mu_n(\gamma) = |\varrho_1(\gamma)|^n \left[c_1(\gamma) \left(\frac{\varrho_1(\gamma)}{|\varrho_1(\gamma)|} \right)^n + \overline{c_1(\gamma)} \left(\frac{\overline{\varrho_1(\gamma)}}{|\varrho_1(\gamma)|} \right)^n \right]$$

• Since the polynomial is quadratic, one can directly handle these expressions

Computational details in the BDF family for k = 3: an upper bound

• For k = 3, the corresponding recursion is

$$(6\gamma + 11)\mu_n(\gamma) - 18\mu_{n-1}(\gamma) + 9\mu_{n-2}(\gamma) - 2\mu_{n-3}(\gamma) = 0 \qquad (n \ge 3)$$

with

$$\mu_0(\gamma) = \frac{6}{6\gamma + 11}, \quad \mu_1(\gamma) = \frac{108}{(6\gamma + 11)^2}, \quad \mu_2(\gamma) = \frac{54(-6\gamma + 25)}{(6\gamma + 11)^3}.$$

• A useful lemma involving a simple root of the function $\mu_n(\cdot)$:

Lemma 3.1 Suppose there exist some $n \in \mathbb{N}^+$ and $\gamma^* > 0$ such that $\mu_n(\gamma^*) = 0$ and $\mu'_n(\gamma^*) \in \mathbb{R} \setminus \{0\}$. Then $\gamma_{\sup} \leq \gamma^*$.

• Let us consider the 6th term

$$\mu_6(\gamma) = \frac{6\left(5184\gamma^4 - 539352\gamma^3 + 4277340\gamma^2 - 7093698\gamma + 3248425\right)}{(6\gamma + 11)^7}$$

The polynomial {5184, -539352, 4277340, -7093698, 3248425} in the numerator has 4 real roots; let $\gamma^* \approx 0.831264$ denote its smallest root (the other three zeros are located at ≈ 1.22747 , ≈ 6.42689 , and ≈ 95.556). Then, due to Lemma 3.1, we have $\gamma_{sup,3} \leq \gamma^*$.

Computational details in the BDF family for k = 3: a lower bound

• It is easily seen from the definition that

 $\exists \gamma_0 > 0 : \mu_n(\gamma_0) \ge 0 \; (\forall n \in \mathbb{N}^+) \implies \gamma_{\sup} \ge \gamma_0.$

- So to finish the proof of $\gamma_{\sup} = \gamma^* \approx 0.831264$ (an algebraic number of degree 4), we verify that $\mu_n(\gamma^*) \ge 0$ for each $n \in \mathbb{N}$
- In this case, the explicit form of $\mu_n(\gamma^*)$ is

$$\mu_n(\gamma^*) = c_1 \varrho_1^n + c_2 \varrho_2^n + \overline{c_2}(\overline{\varrho_2})^n \qquad (n \ge 0),$$

where

• $\rho_1 \approx 0.500518$ is the largest real root of the polynomial

 $P_{\text{BDF31}} = \{34012224, -85030560, 108650160, -91171656, 55033668, -25076142, 8777889, -2366334, 486000, -75816, 10080, -1152, 64\};$

• $\rho_2 \approx 0.312678 + 0.390087i$ is the root of P_{BDF31} with the largest real part;

Computational details in the BDF family for k = 3: final steps of the proof of $\gamma_{sup} = \gamma^* \approx 0.831264$ (an algebraic number of degree 4)

- We take into account that $c_1 \approx 0.50155509$, and $\rho_1 \approx 0.500518$, and $|\rho_2| \approx 0.499935$ (exact algebraic numbers)
- ρ_1 and ρ_2 are close to each other

Now, clearly,
$$\mu_n(\gamma^*) = \varrho_1^n \left[c_1 + c_2 \left(\varrho_2 / \varrho_1 \right)^n + \overline{c_2} \left(\overline{\varrho_2} / \varrho_1 \right)^n \right]$$
, and we have

$$\left| c_2 \left(\frac{\varrho_2}{\varrho_1} \right)^n + \overline{c_2} \left(\frac{\overline{\varrho_2}}{\varrho_1} \right)^n \right| \le 2|c_2| \left| \frac{\varrho_2}{\varrho_1} \right|^n < 2 \cdot \frac{2777}{10000} \left(\frac{9989}{10000} \right)^n.$$

On the other hand,

$$2 \cdot \frac{2777}{10000} \left(\frac{9989}{10000}\right)^n < \frac{50155}{100\,000} < c_1$$

for $n \ge 93$, therefore $\mu_n(\gamma^*) > 0$ for $n \ge 93$.

Finally, one checks that $\mu_n(\gamma^*) > 0$ for $n \in \{0, 1, ..., 92\} \setminus \{6\}$ (recall that $\mu_6(\gamma^*) = 0$), so the proof is complete.

Remark 3.9 We have $\mu_{92}(\gamma^*) \approx 1.585176 \cdot 10^{-28}$.

Computational details in the BDF family for k = 4

• For k = 4, the recursion is

 $(12\gamma + 25)\mu_n(\gamma) - 48\mu_{n-1}(\gamma) + 36\mu_{n-2}(\gamma) - 16\mu_{n-3}(\gamma) + 3\mu_{n-4}(\gamma) = 0 \qquad (n \ge 4)$ with

$$\mu_0(\gamma) = \frac{12}{12\gamma + 25}, \quad \mu_1(\gamma) = \frac{576}{(12\gamma + 25)^2}, \quad \mu_2(\gamma) = \frac{1296(-4\gamma + 13)}{(12\gamma + 25)^3},$$
$$\mu_3(\gamma) = \frac{192\left(144\gamma^2 - 1992\gamma + 2137\right)}{(12\gamma + 25)^4}.$$

This time it turns out that

 $\gamma_{\text{sup},4} \approx 0.486220284043$ is the unique real root of the fifth-degree polynomial {147456, -4065024, 97751296, -178921248, 146499984, -39945535};

Computational details in the BDF family for k = 4: harder to analyze

• Recall Lemma 3.1: a simple root of the function $\mu_n(\cdot)$ for some *n* is an upper bound on γ_{sup}

Remark 3.4 Obtaining the exact value of $\gamma_{\sup,4} \approx 0.48622$ proved to be significantly harder than determining that of $\gamma_{\sup,3}$, because we could not apply Lemma 3.1 to bound $\gamma_{\sup,4}$ from above. The value of $\gamma_{\sup,4}$ was found via a series of numerical experiments. For example, to see $\gamma_{\sup,4} < 0.48625$, one checks that the sequence μ_n in Theorem 1.6 for $1 \leq n \leq 27000$ satisfies

 $\mu_n(48625/100000) < 0 \Longleftrightarrow n \in \{26814, 26875, 26886, 26936, 26947, 26997\}.$

To find all these six indices, we used 16000 digits of precision to evaluate the terms of the recursion $\mu_n(48625/100000)$ —15000 digits would be insufficient. In fact, these experiments led to the formulation of Lemma 3.2.

Computational details in the BDF family for k = 4

- A dominant root of the characteristic polynomial = a root with maximum modulus
- A new observation: if a positive dominant root loses its dominant property at a certain value of the parameter γ^* , then $\gamma_{sup} \leq \gamma^*$. More precisely we have the following *elementary* lemma.

The following lemma will be applied to bound γ_{sup} from above when the characteristic polynomial has a unique pair of complex conjugate roots that are dominant.

Lemma 3.2 Suppose that $z \in \mathbb{C} \setminus \mathbb{R}$ with |z| = 1, $w \in \mathbb{C} \setminus \{0\}$, and a real sequence $v_n \to 0$ $(n \to +\infty)$ are given. Then $wz^n + \bar{w}(\bar{z})^n + v_n < 0$ for infinitely many $n \in \mathbb{N}$.

 The situation becomes much harder to analyze, if there are e.g. 4 dominant complex roots. Many unsolved questions in this area, related to deep theorems in Diophantine approximation. Some recent progress:

- Ouaknine, J., Worrell, J.: Decision problems for linear recurrence sequences. In: reachability problems, 6th International Workshop, RP 2012, Bordeaux, France, September 17–19 (2012). doi:10.1007/978-3-642-33512-9_3
- Ouaknine, J., Worrell, J.: Positivity problems for low-order linear recurrence sequences. In: proceedings of the 25th Annual ACM-SIAM Symposium on Discrete Algorithms (2014). doi:10.1137/1.9781611973402.27
- 13. Ouaknine, J., Worrell, J.: Automata, languages, and programming. Part II: on the positivity problem for simple linear recurrence Sequences, pp. 318–329. Springer, Heidelberg (2014)
- 14. Ouaknine, J., Worrell, J.: Ultimate positivity is decidable for simple linear recurrence sequences, pp. 330-341. Springer, Heidelberg (2014)

Computational details in the BDF family for k = 4: final steps of $\gamma_{sup} = \gamma^* \approx 0.48622$ (a degree 5 algebraic number)

- For k = 4 and $0 < \gamma < \frac{7}{12} \approx 0.5833$, the characteristic polynomial has 2 positive real ($\rho_{1,2}$) and 2 conjugate complex roots ($\rho_{3,4}$), and $0 < \rho_2 < \rho_1$
- Moreover we have
 - $|\varrho_3(\gamma)| = |\varrho_4(\gamma)| < \varrho_1(\gamma)$ for $0 < \gamma < \gamma^*$;
 - $|\varrho_3(\gamma^*)| = |\varrho_4(\gamma^*)| = \varrho_1(\gamma^*)$ for $\gamma = \gamma^*$;
 - $\varrho_1(\gamma) < |\varrho_3(\gamma)| = |\varrho_4(\gamma)|$ for $\gamma^* < \gamma < 7/12$.
- So Lemma 3.2 becomes applicable, and the rest of the proof is similar to the final steps of the proof in the previous *k* = 3 case

Computational details for k = 5

$$(60\gamma + 137)\mu_n(\gamma) - 300\mu_{n-1}(\gamma) + 300\mu_{n-2}(\gamma) - 200\mu_{n-3}(\gamma) + 75\mu_{n-4}(\gamma) - 12\mu_{n-5}(\gamma) = 0 \qquad (n \ge 5)$$

with

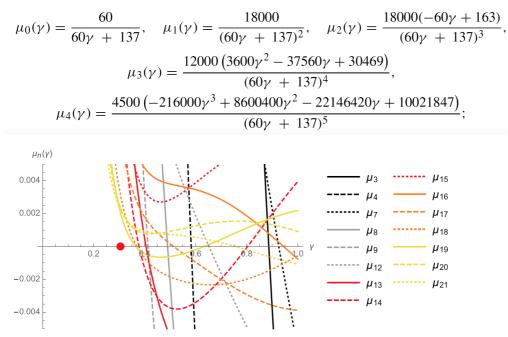


Fig. 1 The functions $\gamma \mapsto \mu_n(\gamma)$ for $1 \le n \le 21$ corresponding to the BDF5 method are shown (the curves with indices $n \in \{1, 2, 5, 6, 10, 11\}$ are not visible in this plot window). The *red dot* is placed at $\gamma = \gamma_{sup.5} \approx 0.30421$

Computational details for k = 5

• $\gamma_{sup,5} \approx 0.304213712525$ is the smaller real root of the tenth-degree polynomial

{918330048000000000,	85812841152000000000,	11922800956027200000000,
-158236459797931200000000,	1300372831455671124000000,	-3469598208824475416400000,
5222219230639370911710000,	-4938342912266137089480000,	2829602902356809601352800,
-897140360120473365541380,	113406532200497326720157};	

Computational details for k = 6

 $3(20\gamma + 49)\mu_n(\gamma) - 360\mu_{n-1}(\gamma) + 450\mu_{n-2}(\gamma) - 400\mu_{n-3}(\gamma) + 225\mu_{n-4}(\gamma) - 400\mu_{n-3}(\gamma) + 225\mu_{n-4}(\gamma) - 400\mu_{n-3}(\gamma) + 400\mu_{n-$

 $72\mu_{n-5}(\gamma) + 10\mu_{n-6}(\gamma) = 0 \qquad (n \ge 6)$

with

$$\mu_0(\gamma) = \frac{20}{20\gamma + 49}, \quad \mu_1(\gamma) = \frac{2400}{(20\gamma + 49)^2},$$
$$\mu_2(\gamma) = \frac{3000(-20\gamma + 47)}{(20\gamma + 49)^3}, \quad \mu_3(\gamma) = \frac{8000(400\gamma^2 - 3440\gamma + 2131)}{3(20\gamma + 49)^4},$$
$$\mu_4(\gamma) = \frac{500(-24000\gamma^3 + 695600\gamma^2 - 1343380\gamma + 474833)}{(20\gamma + 49)^5},$$
$$\mu_5(\gamma) = \frac{160(480000\gamma^4 - 53296000\gamma^3 + 283987200\gamma^2 - 212499240\gamma + 84071653)}{(20\gamma + 49)^6}$$

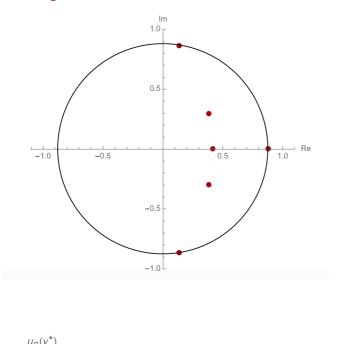
Computational details for k = 6

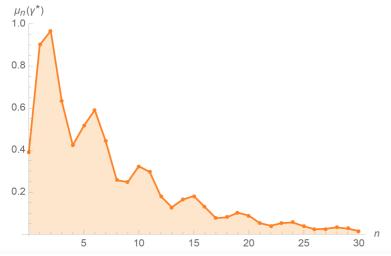
 $\gamma_{sup,6} \approx 0.131359487166$ is the smaller real root of the 18th-degree polynomial

122639585534504839818945201438720000000, 27549570033081885223128023207444584857600000, -3841469418723966761157769983211793789485056000,5587246198359348966734174906666273788289332150272, -17429944795858965010882996868073155329514839408640.-541370800878125712591610585145194659522378896880,

{301499153838045|27552831160320000000, 384963168041618344234237602954215424000000, 688321830171904949334479202088109368934400000, 3383327891741061214240426918034255832010259451480,33328092641186254550760247661168148768262937067}.

Computational details: k = 6





Summary for the BDF and AB families

We have identified two types of conditions that characterize γ_{sup} in these multistep families:

(i) a positive real dominant root of the characteristic polynomial corresponding to the recursion $\mu_n(\gamma)$ loses its dominant property at $\gamma = \gamma_{sup}$, or

(ii) there is an index $n_0 \in \mathbb{N}$ such that γ_{sup} is a simple root of the function $\mu_{n_0}(\cdot)$. It turns out that γ_{sup} is determined

- by condition (i) for the BDF methods with $k \in \{2, 4, 5, 6\}$ steps;
- by condition (ii) with $n_0 = 6$ for the 3-step BDF method;
- by condition (ii) with $n_0 = 2$ for the Adams–Bashforth methods with $k \in \{1, 2, 3\}$ steps.