

Exact optimal values of step-size coefficients for boundedness of linear multistep methods

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Abstract

Linear multistep methods (LMMs) applied to approximate the solution of initial value problems—typically arising from method-of-lines semidiscretizations of partial differential equations—are often required to have certain monotonicity or boundedness properties (e.g. strong-stability-preserving, total-variation-diminishing or total-variation-boundedness properties). These properties can be guaranteed by imposing step-size restrictions on the methods. To qualitatively describe the step-size restrictions, one introduces the concept of step-size coefficient for monotonicity (SCM, also referred to as the strong-stability-preserving (SSP) coefficient) or its generalization, the step-size coefficient for boundedness (SCB). A LMM with larger SCM or SCB is more efficient, and the computation of the maximum SCM for a particular LMM is now straightforward. However, it is more challenging to decide whether a positive SCB exists, or determine if a given positive number is a SCB. Theorems involving sign conditions on certain linear recursions associated to the LMM have been proposed in the literature that allow us to answer the above questions: the difficulty with these theorems is that there are in general infinitely many sign conditions to be verified. In this work we present methods to rigorously check the sign conditions. As an illustration, we confirm some recent numerical investigations concerning the existence of positive SCBs in the BDF and in the extrapolated BDF (EBDF) families. As a stronger result, we determine the optimal values of the SCBs as exact algebraic numbers in the BDF family (with $1 \leq k \leq 6$ steps) and in the Adams–Bashforth family (with $1 \leq k \leq 3$ steps).

Keywords: linear multistep methods, strong stability preservation, step-size coefficient for monotonicity, step-size coefficient for boundedness.

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1 Introduction

Let us consider an initial-value problem

$$u'(t) = F(u(t)) \text{ for } t \geq 0, \text{ with } u(0) = u_0, \quad (1)$$

where $F : \mathbb{V} \rightarrow \mathbb{V}$ is a given function, $u_0 \in \mathbb{V}$ is a given initial value in some vector space \mathbb{V} , and u denotes the unknown function. In applications it is often crucial for the numerical solution u_n to satisfy certain monotonicity or boundedness properties.

Example 1.1. *Many important partial differential equations have the property that they preserve*

- (i) *the interval containing the initial data;*
- (ii) *or, as a special case, non-negativity of the initial data.*

For example, if one considers a scalar hyperbolic conservation law with initial condition $U(x, t_0) \in [U_{\min}, U_{\max}]$ with some constants $U_{\min} \leq U_{\max}$ for $x \in \mathbb{R}$, then it is known that the solution satisfies $U(x, t) \in [U_{\min}, U_{\max}]$ for $x \in \mathbb{R}$ and $t \geq t_0$. To approximate the solution U of this partial differential equation, one often uses a method-of-lines semidiscretization in space, and obtains a system of ordinary differential equations (1). For many semidiscretizations, the initial-value problem (1) also preserves (i) or (ii). Finally, one typically uses a Runge–Kutta method or a linear multistep method to discretize (1): in this setting it is natural to require that the time discretization u_n should also preserve (i) or (ii).

In situations when the numerical method is a linear multistep method (LMM) approximating the solution of (1), the boundedness property can be expressed as

$$\|u_n\| \leq \mu \cdot \max_{0 \leq j \leq k-1} \|u_j\| \quad (n \geq k), \quad (2)$$

where the constant $\mu \geq 1$ is independent of n , the starting vectors u_j ($0 \leq j \leq k-1$) and the problem (1); μ is determined only by the LMM. The monotonicity property, or strong-stability-preserving (SSP) property, is recovered if (2) holds with $\mu = 1$. Common choices for the seminorm $\|\cdot\|$ on \mathbb{V} in applications include the supremum norm or the total variation seminorm. For LMMs, a more detailed exposition of the above topics together with references can be found, for example, in [16, Section 1]. For Runge–Kutta methods, analogous questions have been analyzed thoroughly and solved satisfactorily in [8]. In what follows, we focus on LMMs.

In the literature a considerable amount of work has been done on developing conditions that guarantee (2). One possibility is to impose some restrictions on the step size Δt of the LMM. These restrictions lead to the concepts of step-size coefficient for monotonicity (SCM) and step-size coefficient for boundedness (SCB)—see Definitions 1.4 and 1.5 below. Depending on the context, the SCM is also referred to as the strong-stability-preserving (SSP) coefficient. The SCB is a generalization of the SCM: for many practically important LMMs, there is no positive SCM, while a positive SCB still exists. It is thus natural to ask whether a positive step-size coefficient (SCM or SCB) exists for a particular LMM, or

determine if a given positive number is a step-size coefficient. Since a LMM with larger step-size coefficient is more efficient, one is also interested in the maximum value of the SCM or SCB. Conditions that are easy to check and are necessary and sufficient for the existence of a positive SCM, or for a given positive number to be a SCM have already been devised, see [16, Section 1.1].

However, even for a single LMM, it seems more difficult

- (i) to decide whether a positive SCB exists;
- (ii) to determine if a given positive number is a SCB;
- (iii) to compute the maximum SCB.

In the rest of the paper, we pursue these goals. The theoretical framework we use is presented in [9, 16], while the computational techniques we apply show many similarities with those of [10]. All computations in this work have been performed by using *Mathematica* 10.

The structure of our paper is as follows. In Section 1.1 we present some definitions and notation. In Sections 1.2 and 1.3 we review the main results of [9] and [16] concerning (ii) and (i) above, respectively. Section 2 contains our theorems for three families of multistep methods:

- for the extrapolated BDF (EBDF) methods we answer (i);
- for the BDF methods (as implicit methods) we answer (iii);
- for the Adams–Bashforth (AB) methods (as explicit methods) we answer (iii).

The proofs are described in Section 3.

Remark 1.2. *In our proofs we essentially need to establish the non-negativity of certain (parametric) linear recursions. Recently, some general results have been devised solving the problem of (ultimate) positivity in several classes of integer linear recursions, see, for example, the series of papers [11, 12, 13, 14].*

1.1 Preliminaries and notation

A LMM has the form

$$u_n = \sum_{j=1}^k a_j u_{n-j} + \Delta t \sum_{j=0}^k b_j F(u_{n-j}) \quad (n \geq k), \quad (3)$$

where $k \geq 1$, the step number of the LMM, is a fixed integer, and the coefficients $a_j, b_j \in \mathbb{R}$ determine the method. The step size of the method $\Delta t > 0$ is assumed to be fixed, and we suppose that the starting values for the LMM, u_0 (appearing in (1)) and u_j ($1 \leq j \leq k-1$), are also given. The quantity u_n approximates the exact solution value $u(n\Delta t)$. The generating polynomials associated with the LMM are denoted by

$$\rho(\zeta) := \zeta^k - \sum_{j=1}^k a_j \zeta^{k-j} \quad \text{and} \quad \sigma(\zeta) := \sum_{j=0}^k b_j \zeta^{k-j}. \quad (4)$$

A non-constant univariate polynomial is said to satisfy the *root condition*, if all of its roots have absolute value ≤ 1 , and any root with absolute value $= 1$ has multiplicity one. As in [16], the LMMs in this work are also required to satisfy the following basic assumptions.

1. $\sum_{j=1}^k a_j = 1$ and $\sum_{j=1}^k ja_j = \sum_{j=0}^k b_j$ (consistency).
 2. The polynomial ρ satisfies the root condition (zero-stability).
 3. The polynomials ρ and σ have no common root (irreducibility).
 4. $b_0 \geq 0$.
- (5)

All well-known methods used in practice satisfy the four conditions in (5).

The *stability region* of the LMM, denoted by \mathcal{S} , is defined as

$$\mathcal{S} := \{\lambda \in \mathbb{C} : 1 - \lambda b_0 \neq 0 \text{ and } \rho - \lambda\sigma \text{ satisfies the root condition}\},$$

see [16, Section 2.1]. The interior of the stability region will be denoted by $\text{int}(\mathcal{S})$.

Remark 1.3. Notice that the above definition of the stability region \mathcal{S} is slightly more restrictive than the usual one. The usual definition of the stability region (see, for example, in [4]),

$$\tilde{\mathcal{S}} := \{\lambda \in \mathbb{C} : \rho - \lambda\sigma \text{ satisfies the root condition}\},$$

does not exclude the case of a vanishing leading coefficient of the polynomial $\mathcal{P}(\cdot, \lambda) := \rho(\cdot) - \lambda\sigma(\cdot)$. With this definition $\tilde{\mathcal{S}}$, one can construct simple examples with the following properties:

- the order of the recurrence relation generated by the LMM becomes $< k$ for certain values of the step size $\Delta t > 0$, hence k starting values of the LMM cannot be chosen arbitrarily;
- there is an isolated point of the boundary of $\tilde{\mathcal{S}}$ (being an element of $\tilde{\mathcal{S}}$);
- the boundary of $\tilde{\mathcal{S}}$ is not a subset of the root locus curve due to these isolated boundary points.

Similarly, in the class of multiderivative multistep methods (being a generalization of LMMs), it seems advantageous to exclude the values of $\lambda \in \mathbb{C}$ from the definition of the stability region for which the leading coefficient of the corresponding polynomial $\mathcal{P}(\cdot, \lambda)$ vanishes.

The set of natural numbers $\{0, 1, \dots\}$ is denoted by \mathbb{N} , while the complex conjugate of z is \bar{z} . The *dominant root* of a non-constant univariate polynomial is any root having the largest absolute value.

When we define algebraic numbers in later sections, a polynomial

$$\sum_{j=0}^n a_j x^j \text{ with } a_j \in \mathbb{Z}, a_n \neq 0 \text{ and } n \geq 3$$

will be represented simply by its coefficient list

$$\{a_n, a_{n-1}, \dots, a_0\}. \quad (6)$$

Now we recall the definition of the *step-size coefficient for boundedness* and *monotonicity*, respectively, corresponding to a given linear multistep method.

Definition 1.4. *Suppose that the method coefficients $a_j \in \mathbb{R}$ ($1 \leq j \leq k$) and $b_j \in \mathbb{R}$ ($0 \leq j \leq k$) satisfy (5). We say that $\gamma > 0$ is a step-size coefficient for boundedness (SCB) of the corresponding LMM, if $\exists \mu \geq 1$ such that*

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

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

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

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

Definition 1.5. *We say that $\gamma > 0$ is a step-size coefficient for monotonicity (SCM) of the LMM, if Definition 1.4 holds with $\mu = 1$.*

Given a LMM, the following abbreviations will be used throughout this work:

- $\exists \text{SCM} > 0$ and $\nexists \text{SCM} > 0$ to indicate that there is a positive / there is no positive step-size coefficient for monotonicity, respectively;
- $\exists \text{SCB} > 0$ and $\nexists \text{SCB} > 0$ to indicate that there is a positive / there is no positive step-size coefficient for boundedness, respectively.

It is clear from Definitions 1.4-1.5 that for a given LMM

$$\exists \text{SCM} > 0 \implies \exists \text{SCB} > 0.$$

If $\exists \text{SCB} > 0$, then we define

$$\gamma_{\text{sup}} := \sup\{\gamma > 0 : \gamma \text{ is a SCB}\}.$$

When a family of k -step LMMs is given, sometimes we will use the symbol $\gamma_{\text{sup},k}$ instead.

1.2 A necessary and sufficient condition for $\gamma > 0$ to be a SCB

Let us fix a particular LMM. For a given $\gamma \in \mathbb{R}$, we define an auxiliary sequence $\mu_n(\gamma)$ ($n \in \mathbb{Z}$) as in [16, (2.10)] by

$$\mu_n(\gamma) := \begin{cases} 0 & \text{for } n < 0, \\ b_n - \gamma b_0 \mu_n(\gamma) + \sum_{j=1}^k (a_j - \gamma b_j) \mu_{n-j}(\gamma) & \text{for } 0 \leq n \leq k, \\ -\gamma b_0 \mu_n(\gamma) + \sum_{j=1}^k (a_j - \gamma b_j) \mu_{n-j}(\gamma) & \text{for } n > k. \end{cases} \quad (7)$$

The following characterization appears in [16, Theorem 2.2].

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

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

The above theorem is based on the material developed in [9]. In [9, Section 6], the authors numerically determine the maximum SCB values for members of several parametric families of LMMs by repeatedly applying the following test. For a particular LMM and given $\gamma > 0$, they check if γ is a SCB by choosing a large $N \in \mathbb{N}$, and verifying $\mu_n(\gamma) \geq 0$ for all $1 \leq n \leq N$. However, as the authors point out in [9], it is not obvious (neither *a priori* nor *a posteriori*) how large N one should choose to conclude—with high certainty—that $\mu_n(\gamma) \geq 0$ for all $n \in \mathbb{N}^+$. They typically use $N \approx 10^3$; as a comparison, see our Remark 3.4.

1.3 The existence of a SCB

For a fixed LMM and given $\gamma > 0$, Theorem 1.6 provides a necessary and sufficient condition for γ to be a SCB. But to decide—with the help of this theorem—whether \exists SCB > 0 , one should check condition (8) for infinitely many $\gamma > 0$ values, and for each γ , there are infinitely many sign conditions $\mu_n(\gamma) \geq 0$ to be verified.

To overcome this difficulty, [16, Theorem 3.1] combines Theorem 1.6 with the results of [1] to present some *simpler* conditions that are *almost* necessary and sufficient for \exists SCB > 0 . “Almost” in the previous sentence means that the conditions in [16, Theorem 3.1] are necessary and sufficient for \exists SCB > 0 (not in the full, but) in a slightly restricted class of LMMs; and “simpler” means that these conditions do not involve the parametric recursion $\mu_n(\gamma)$ in (7), rather, a non-parametric recursion τ_n determined by the method coefficients as

$$\tau_n := \begin{cases} 0 & \text{for } n < 0, \\ b_n + \sum_{j=1}^k a_j \tau_{n-j} & \text{for } 0 \leq n \leq k, \\ \sum_{j=1}^k a_j \tau_{n-j} & \text{for } n > k. \end{cases} \quad (9)$$

Since we will not work with [16, Theorem 3.1] directly, here we cite only [16, Corollary 3.3].

Corollary 1.7. *Suppose the LMM satisfies (5). We define*

$$n_0 := \min\{n : 1 \leq n \leq k \text{ and } \tau_n \neq 0\}. \quad (10)$$

(i) *If $\tau_n > 0$ for all $n \geq n_0$, and the only root of the polynomial ρ appearing in (4) with modulus 1 is 1, then $\exists \text{ SCB} > 0$.*

(ii) *If $\tau_n \leq 0$ for some $n \geq n_0$ being a multiple of n_0 , then $\nexists \text{ SCB} > 0$.*

The index n_0 defined above can be shown to exist due to consistency and zero-stability of the LMM.

As an application of [16, Theorem 3.1] or Corollary 1.7, [16, Section 5] analyzes some well-known classical LMMs, including

- the Adams–Moulton (or implicit Adams),
- the Adams–Bashforth (or explicit Adams),
- the BDF,
- the extrapolated BDF (EBDF),
- the Milne–Simpson and
- the Nyström methods.

These investigations confirm and extend some earlier results [5, 6, 7, 9] concerning the existence of step-size coefficients for monotonicity or step-size coefficients for boundedness. The results of [16, Section 5] have the following form.

Consider a discrete family of LMMs from the previous paragraph, parametrized by the step number $k \in \mathbb{N}$. Let $1 \leq k_{\min} \leq k_{\max} \leq +\infty$ denote some fixed bounds on k coming from practical considerations (e.g. zero-stability of the LMM), that is, we consider the step numbers $k_{\min} \leq k \leq k_{\max}$. Then there exist two integers $0 \leq k_{\text{mon}} \leq k_{\text{bdd}}$ such that

- $\exists \text{ SCM} > 0 \iff k_{\min} \leq k \leq k_{\text{mon}}$;
- $(\nexists \text{ SCM} > 0 \text{ and } \exists \text{ SCB} > 0) \iff k_{\text{mon}} + 1 \leq k \leq k_{\text{bdd}}$;
- $\nexists \text{ SCB} > 0 \iff k_{\text{bdd}} + 1 \leq k \leq k_{\max}$.

It is to be understood that if $\ell_1 \leq k \leq \ell_2$ with $\ell_1 > \ell_2$ in any of the inequalities above, then the corresponding case does not occur. Some examples from [16, Section 5] are provided in the table below.

LMM family	k_{\min}	k_{\max}	k_{mon}	k_{bdd}
Adams–Bashforth	1	$+\infty$	1	3
BDF	1	6	1	6
EBDF	1	6	1	5
Milne–Simpson	2	$+\infty$	1	1

Out of the several LMMs investigated in [16, Section 5], there are however two families—the BDF methods with $3 \leq k \leq 6$ steps, and the EBDF methods with $3 \leq k \leq 5$ steps—for which the corresponding inequalities

$$\tau_n > 0 \quad \text{for } n \geq n_0 \tag{11}$$

appearing in Corollary 1.7 are not verified completely. More precisely, (11) is verified only up to a finite value $n_0 \leq n \leq N$ (for example, up to $N = 500$), and it is observed that, for these large n values, τ_n is already close enough to $\lim_{n \rightarrow +\infty} \tau_n = 1$ to conclude (“we have no formal proof . . . , but convincing numerical evidence instead”) the validity of (11) (see [16, Conclusions 5.3 and 5.4]).

2 Main results

2.1 Positivity of the τ_n sequences in the EBDF family

Theorem 2.1. *Let us fix any $3 \leq k \leq 5$ and consider the EBDF family with k steps. Then the sequence τ_n satisfies $\tau_n > 0$ for $n \geq n_0 = 1$ (see (9) and (10)).*

The above theorem completes and verifies the numerical proof of [16, Conclusion 5.4] regarding the EBDF methods with $k \in \{3, 4, 5\}$ steps. In the proof of Theorem 2.1, given in Sections 3.1 and 3.4, we explicitly represent τ_n as a linear combination of powers of algebraic numbers to estimate this sequence from below and hence prove its positivity.

As a combination of [16, Conclusion 5.4] and our Theorem 2.1 we obtain the following result.

Corollary 2.2. *In the EBDF family*

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

2.2 Exact optimal SCB values in the BDF family

We complete the numerical proof of [16, Conclusion 5.3] concerning the existence of SCB for the BDF methods with $3 \leq k \leq 6$ steps. However, instead of just proving the positivity of the corresponding sequences τ_n , we directly determine the exact and optimal values of the SCB constants for $2 \leq k \leq 6$. For the sake of completeness, the $k = 1$ case (the implicit Euler method) is also included. The approximate numerical values of $\gamma_{\text{sup},k}$ below have been rounded down. The polynomial coefficients—see (6) for the notation—corresponding to the cases $k = 5$ and $k = 6$ have been aligned for easier readability (and they are to be read in the usual way, horizontally from left to right).

Theorem 2.3. *The optimal values of the step-size coefficients for boundedness $\gamma_{\text{sup},k}$ in the BDF family are given by the following exact algebraic numbers:*

- $\gamma_{\text{sup},1} = +\infty$;
- $\gamma_{\text{sup},2} = 1/2$;
- $\gamma_{\text{sup},3} \approx 0.831264155297$ is the smallest real root of the 4th-degree polynomial

$$\{5184, -539352, 4277340, -7093698, 3248425\};$$

- $\gamma_{\text{sup},4} \approx 0.486220284043$ is the unique real root of the 5th-degree polynomial

$$\{147456, -4065024, 97751296, -178921248, 146499984, -39945535\};$$

- $\gamma_{\text{sup},5} \approx 0.304213712525$ is the smaller real root of the 10th-degree polynomial

$$\begin{aligned} &\{9183300480000000000, && 85812841152000000000, && 11922800956027200000000, \\ &-158236459797931200000000, && 1300372831455671124000000, && -3469598208824475416400000, \\ &5222219230639370911710000, && -4938342912266137089480000, && 2829602902356809601352800, \\ &-897140360120473365541380, && 113406532200497326720157\}; \end{aligned}$$

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

$$\begin{aligned} &\{301499153838045275528311603200000000, && 122639585534504839818945201438720000000, \\ &384963168041618344234237602954215424000000, && 27549570033081885223128023207444584857600000, \\ &688321830171904949334479202088109368934400000, && -3841469418723966761157769983211793789485056000, \\ &114843588487750902323103668249803599786305126400, && -1006269459507863531788997342497299304467812843520, \\ &5587246198359348966734174906666273788289332150272, && -17429944795858965010882996868073155329514839408640, \\ &35959114141443095864886240750517884787497897431040, && -53357827225132542443145327442029250536098863687680, \\ &58779078470720235677143648519968524504336318905600, && -48117131040654192740877887801688549303578668712064, \\ &28809153195856173726312967696976168633917662024240, && -12158530101520566099221248226347019432756062262240, \\ &3383327891741061214240426918034255832010259451480, && -541370800878125712591610585145194659522378896880, \\ &33328092641186254550760247661168148768262937067\}. \end{aligned}$$

The proofs of the above results are given in Sections 3.2 and 3.5. From a technical point of view, the proof of the $k = 3$ case is different from the other cases, see Remark 3.5.

2.3 Exact optimal SCB values in the Adams–Bashforth family

To further illustrate our techniques, we have computed the largest SCB values for an explicit LMM family as well; we chose the Adams–Bashforth methods with $1 \leq k \leq 4$ steps.

For $k = 1$ (i.e. for the explicit Euler method) it is known ([16, Theorem 5.2]) that $\exists \text{SCM} > 0$, hence $\exists \text{SCB} > 0$.

For any $k \geq 4$, [16, Theorem 5.2] proves—with the help of the sequence τ_n —that $\nexists \text{SCB} > 0$. The reason we include the $k = 4$ case here is to show an example of using the parametric sequence $\mu_n(\gamma)$ and Theorem 1.6 instead of τ_n in Corollary 1.7 (ii) to detect $\nexists \text{SCB} > 0$.

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:*

- $\gamma_{\text{sup},1} = 1$;

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

The proofs of these results are found in Sections 3.3 and 3.6.

3 Proofs

3.1 Summary of the proof techniques for the EBDF methods

The proofs in Section 3.4 for the EBDF methods use the following argument. Since τ_n in (9) is a solution of a linear recursion, it is represented as

$$\tau_n = \sum_{j=1}^k c_j \varrho_j^n, \quad (12)$$

where the quantities $\varrho_j \in \mathbb{C}$ are the roots of the corresponding characteristic polynomial (without multiple roots for each EBDF method), and the constants $c_j \in \mathbb{C}$ are determined by the starting values. By bounding $|c_j|$ and $|\varrho_j|$, we prove the inequality $\tau_n > 0$ for all $n \geq 1$.

3.2 Summary of the proof techniques for the BDF methods

The proofs in Section 3.5 for the BDF methods are based on the following. For any given $\gamma > 0$, the linear recursion (7) takes the form

$$\sum_{j=0}^k c_j(\gamma) \mu_{n-j}(\gamma) = 0 \quad (k \leq n \in \mathbb{N}), \quad (13)$$

where the coefficients $c_j(\gamma)$ ($0 \leq j \leq k$) and the starting values $\mu_j(\gamma)$ ($0 \leq j \leq k-1$) are determined by the LMM. The corresponding characteristic polynomial is denoted by

$$\mathcal{P}_k(\varrho, \gamma) := \sum_{j=0}^k c_j(\gamma) \varrho^{k-j}. \quad (14)$$

We apply the characterization in Theorem 1.6 together with Observations 1-4 presented below. Lemma 3.1 and Lemma 3.2 will be used to bound γ_{sup} from above for the k -step BDF methods with $k = 3$ and $k \in \{2, 4, 5, 6\}$, respectively. Then, by using representations similar to (12) and Observation 4, we show in each case that the proposed upper bound for γ_{sup} is sharp.

- **Observation 1**

For a k -step BDF method ($1 \leq k \leq 6$), it is known [4] that $-\gamma \in \text{int}(\mathcal{S})$ for any $\gamma > 0$. Therefore, the condition (8) in Theorem 1.6 reduces to $\mu_n(\gamma) \geq 0$ ($n \in \mathbb{N}^+$).

• **Observation 2**

It is easily seen from Definition 1.4 that if $\gamma_0 > 0$ is a SCB, then each number from the interval $(0, \gamma_0]$ is also a SCB; thus, by (8), we also have $\mu_n(\gamma) \geq 0$ for all $n \in \mathbb{N}^+$ and $\gamma \in (0, \gamma_0]$. Since the function $\gamma \mapsto \mu_n(\gamma)$ (clearly being a rational function for any fixed $n \in \mathbb{N}$ due to the form of the linear recursion (7)) cannot be non-negative in a neighborhood of a simple zero, we immediately obtain the following upper bound on γ_{sup} (in the lemma, μ'_n denotes the derivative 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 $\gamma_{\text{sup}} \leq \gamma^*$.*

• **Observation 3**

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 $\nu_n \rightarrow 0$ ($n \rightarrow +\infty$) are given. Then $wz^n + \bar{w}(\bar{z})^n + \nu_n < 0$ for infinitely many $n \in \mathbb{N}$.*

Proof. We introduce $\varphi, \psi \in [0, 2\pi)$ via the relations $z = \exp(i\varphi)$ and $w = |w| \exp(i\psi)$. Due to symmetry, we can suppose that $\varphi \in (0, \pi)$, so there is a $\delta \in (0, \pi/2)$ such that $\delta < \varphi < \pi - \delta$. Then

$$wz^n + \bar{w}(\bar{z})^n + \nu_n = 2|w| \cos(n\varphi + \psi) + \nu_n. \quad (15)$$

We show that

$$\cos(n\varphi + \psi) \leq \cos(\pi/2 + \delta/2) \text{ for infinitely many } n. \quad (16)$$

Indeed, the inequality in (16) holds if and only if $n \in \mathbb{N}$ and $k \in \mathbb{Z}$ are chosen such that

$$\text{LHS} := (\pi/2 + \delta/2 - \psi + 2\pi k)/\varphi \leq n \leq (3\pi/2 - \delta/2 - \psi + 2\pi k)/\varphi =: \text{RHS}. \quad (17)$$

But $\text{RHS} - \text{LHS} = (\pi - \delta)/\varphi > 1$, so, by taking $k \in \mathbb{N}$ larger and larger, we see that there are infinitely many $n \in \mathbb{N}$ satisfying (17). Finally, by using $|w| \neq 0$, (16), $\cos(\pi/2 + \delta/2) < 0$ and $\nu_n \rightarrow 0$, we get that (15) is also negative for infinitely many n indices. \square

• **Observation 4**

By taking into account the first sentence of Observation 2, we get the following lower bound.

$$\exists \gamma_0 > 0 : \mu_n(\gamma_0) \geq 0 \ (\forall n \in \mathbb{N}^+) \implies \gamma_{\text{sup}} \geq \gamma_0. \quad (18)$$

Remark 3.3. *Notice the similarities between Lemma 3.1 and [2, Lemma 4.5], and between Lemma 3.2 and [2, Lemma 3.1]. Also compare Lemma 3.2 and [16, Theorem 4.3].*

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

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

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.

Remark 3.5. *Regarding the determination of $\gamma_{\text{sup},3}$, the characteristic polynomial $\mathcal{P}_3(\cdot, \gamma)$ has one real root $\varrho_1(\gamma) > 0$ and a pair of complex conjugate roots $\varrho_{2,3}(\gamma)$ with $|\varrho_1(\gamma)| = |\varrho_2(\gamma)| = |\varrho_3(\gamma)|$ for $\gamma = 5/6 \approx 0.83333$. From Lemma 3.2 we would get the bound $\gamma_{\text{sup},3} \leq 5/6$, but this bound is not sharp. However, Lemma 3.1 with $n = 6$ yields the exact value of $\gamma_{\text{sup},3} \approx 0.83126$.*

3.3 Summary of the proof techniques for the Adams–Bashforth methods

Since these LMMs are explicit, we have $b_0 = 0$ in (3), so from (7) we see that for any $n \in \mathbb{N}$ the function $\gamma \mapsto \mu_n(\gamma)$ is a polynomial and $\mu_0(\gamma) = 0$. For $1 \leq k \leq 3$, we study the roots of these polynomials $\mu_n(\cdot)$ for small n to conjecture the value of $\gamma_{\text{sup},k}$. Of course, Observation 1 from the previous section cannot be applied now, because we have to take into account the condition $-\gamma \in \text{int}(\mathcal{S})$ in (8) as well. So we use Lemma 3.1 together with

$$(\exists \gamma_0 > 0 : -\gamma_0 \in \text{int}(\mathcal{S}) \text{ and } \mu_n(\gamma_0) \geq 0 (\forall n \in \mathbb{N}^+)) \implies \gamma_{\text{sup}} \geq \gamma_0 \quad (19)$$

to verify that the conjectured γ_{sup} is indeed the optimal SCB.

Remark 3.6. *For $2 \leq k \leq 3$, it turns out that the dominant root of the characteristic polynomial $\mathcal{P}_k(\cdot, \gamma)$ in (14) is positive real for $\gamma = \gamma_{\text{sup},k}$, so in these cases a result similar to Lemma 3.2 is not applicable.*

3.4 Proofs for the EBDF methods

The coefficients for the EBDF methods are listed, for example, in [15].

3.4.1 The EBDF3 method

For this method, the recursion (9) takes the form

$$11\tau_n - 18\tau_{n-1} + 9\tau_{n-2} - 2\tau_{n-3} = 0 \quad (n \geq 4) \quad (20)$$

with

$$\tau_1 = 18/11, \quad \tau_2 = 126/121, \quad \tau_3 = 1212/1331.$$

We have $\tau_0 = 0$ and $n_0 = 1$, hence it is enough to prove $\tau_n > 0$ for all $n \geq 1$. One root of the characteristic polynomial corresponding to (20) is 1, so we get the representation

$$\tau_n = 1 + \left(\frac{7}{22} + \frac{i\sqrt{39}}{22} \right)^n + \left(\frac{7}{22} - \frac{i\sqrt{39}}{22} \right)^n \quad (n \geq 1).$$

But for $n \geq 1$ we have

$$\left| \frac{7}{22} + \frac{i\sqrt{39}}{22} \right|^n + \left| \frac{7}{22} - \frac{i\sqrt{39}}{22} \right|^n = 2 \cdot \left(\frac{2}{11} \right)^{n/2} \leq 9/10,$$

and the positivity of $\tau_n > 0$ follows.

3.4.2 The EBDF4 method

The recursion (9) now reads

$$25\tau_n - 48\tau_{n-1} + 36\tau_{n-2} - 16\tau_{n-3} + 3\tau_{n-4} = 0 \quad (n \geq 5)$$

with

$$\tau_1 = 48/25, \quad \tau_2 = 504/625, \quad \tau_3 = 10992/15625, \quad \tau_4 = 366516/390625.$$

We again have $\tau_0 = 0$ and $n_0 = 1$. The explicit form of the sequence is

$$\tau_n = 1 + \sum_{j=1}^3 \varrho_j^n \quad (n \geq 1),$$

where $\varrho_1 \in \mathbb{R}$ and $\varrho_{2,3} \in \mathbb{C} \setminus \mathbb{R}$ are the three roots of the cubic polynomial $\{25, -23, 13, -3\}$. This time we have for $n \geq 3$ that

$$\sum_{j=1}^3 |\varrho_j|^n \leq 3 \cdot (3/5)^n \leq 9/10,$$

proving $\tau_n > 0$ for $n \geq 1$.

3.4.3 The EBDF5 method

For this method, the recursion (9) is

$$137\tau_n - 300\tau_{n-1} + 300\tau_{n-2} - 200\tau_{n-3} + 75\tau_{n-4} - 12\tau_{n-5} = 0 \quad (n \geq 6)$$

with

$$\begin{aligned} \tau_1 &= 300/137, & \tau_2 &= 7800/18769, & \tau_3 &= 1271400/2571353, \\ \tau_4 &= 415574100/352275361, & \tau_5 &= 64978409160/48261724457. \end{aligned}$$

We have $\tau_0 = 0$ and $n_0 = 1$. The explicit form of the sequence is

$$\tau_n = 1 + \sum_{j=1}^4 \varrho_j^n \quad (n \geq 1),$$

where $\varrho_{1,2,3,4} \in \mathbb{C} \setminus \mathbb{R}$ are the four roots of the polynomial $\{137, -163, 137, -63, 12\}$. But $|\varrho_{1,2,3,4}| \leq 71/100$, so for $n \geq 5$ we have

$$\sum_{j=1}^4 |\varrho_j|^n \leq 4 \cdot (71/100)^n \leq 9/10,$$

proving $\tau_n > 0$ for $n \geq 1$.

3.5 Proofs for the BDF methods

The coefficients for the BDF methods are listed, for example, in [4].

3.5.1 The BDF1 method

We include this method here for the sake of completeness. The recursion (13) now has the form

$$(\gamma + 1)\mu_n(\gamma) - \mu_{n-1}(\gamma) = 0 \quad (n \geq 1)$$

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 $\gamma > 0$.

3.5.2 The BDF2 method

The recursion (13) takes the form

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

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

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

with a suitable $c_1(\gamma) \in \mathbb{C} \setminus \{0\}$ and $\varrho_1(\gamma) \in \mathbb{C} \setminus \mathbb{R}$. Due to Lemma 3.2 with $\nu_n \equiv 0$, the expression in [...] is negative for infinitely many n . Hence, by Theorem 1.6, $1/2 + \varepsilon$ is not a SCB for any $\varepsilon > 0$, implying $\gamma_{\text{sup},2} < 1/2 + \varepsilon$.

Conversely, by verifying $\mu_n(1/2) = 2^{-n-1}(n+1) \geq 0$ for all $n \in \mathbb{N}$ and taking into account (18), we see that $\gamma_{\text{sup},2} \geq 1/2$, so the proof is complete.

3.5.3 The BDF3 method

The recursion (13) is

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

with

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

Let us consider the term

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

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 3 zeros are located at ≈ 1.22747 , ≈ 6.42689 and ≈ 95.556). Then, due to Lemma 3.1, we have $\gamma_{\text{sup},3} \leq \gamma^*$.

To complete the proof, we show that $\mu_n(\gamma^*) \geq 0$ ($\forall n \in \mathbb{N}$), meaning that $\gamma_{\text{sup},3} \geq \gamma^*$ by (18). Indeed, for $\gamma = \gamma^*$, the explicit form of the recursion is

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

where

- $\varrho_1 \approx 0.500518$ is the largest real root of the polynomial

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

- $\varrho_2 \approx 0.312678 + 0.390087i$ is the root of P_{BDF31} with the largest real part;
- $c_1 \approx 0.50155509$ is the largest real root of the polynomial

$$P_{\text{BDF32}} := \{91221089034315373632, -76017574195262811360, 26664298621295150160, -9975778735584785400, 2799915334883820972, -498764709912473586, 93247136355378087, -8606361446997984, 425210419226880, -10041822761472, 76685377536, -237993984, 262144\};$$

- $c_2 \approx -0.0631319 - 0.270418i$ is the root of P_{BDF32} with the smallest real part.

Remark 3.7. The 12th-degree algebraic numbers $\varrho_{1,2}$ are of course roots of the cubic characteristic polynomial (14), with γ replaced by the 4th-degree algebraic number γ^* ; that is, $\mathcal{P}_3(\varrho_{1,2}, \gamma^*) = 0$.

Remark 3.8. Notice that $|\varrho_2| \approx 0.499935$ is relatively close to $|\varrho_1| \approx 0.500518$. This results in an increased computational cost needed to finish the proof (cf. Remark 3.5).

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

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

On the other hand,

$$2 \cdot \frac{2777}{10000} \left(\frac{9989}{10000} \right)^n < \frac{50155}{100000} < c_1$$

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

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

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

3.5.4 The BDF4 method

The recursion (13) is

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

with

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

For $\gamma > 0$, the characteristic polynomial of the recursion, $\mathcal{P}_4(\cdot, \gamma)$, has multiple roots if and only if $\gamma = 7/12 \approx 0.5833$. In the rest of the proof, it will be sufficient to focus on the interval $0 < \gamma < 7/12$.

For any $0 < \gamma < 7/12$, let us denote the four distinct roots of $\mathcal{P}_4(\cdot, \gamma)$ by $\varrho_{1,2,3,4}(\gamma)$. Then $0 < \varrho_2(\gamma) < \varrho_1(\gamma) < 1$ and $\varrho_{3,4}(\gamma) \in \mathbb{C} \setminus \mathbb{R}$. Let us denote by

$$\gamma^* \approx 0.48622 \tag{21}$$

the 5th-degree algebraic number listed in the row of $\gamma_{\text{sup},4}$ in Theorem 2.3. By separating the real and imaginary parts of $\mathcal{P}_4(x + iy, \gamma)$, then setting up and solving the appropriate system of polynomial equations over the reals, we can prove that

- $|\varrho_3(\gamma)| = |\varrho_4(\gamma)| < \varrho_1(\gamma)$ 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 $\gamma^* < \gamma < 7/12$.

In other words, the positive real root $\varrho_1(\gamma)$ is no longer dominant for $\gamma > \gamma^*$.

First we prove $\gamma_{\text{sup},4} \geq \gamma^*$ by proving $\mu_n(\gamma^*) > 0$ ($\forall n \in \mathbb{N}$), see (18). For $\gamma = \gamma^*$ we have the representation

$$\mu_n(\gamma^*) = c_1(\gamma^*) (\varrho_1(\gamma^*))^n + c_2(\gamma^*) (\varrho_2(\gamma^*))^n + c_3(\gamma^*) (\varrho_3(\gamma^*))^n + \overline{c_3(\gamma^*)} (\overline{\varrho_3(\gamma^*)})^n \quad (n \geq 0),$$

where

- $\varrho_1(\gamma^*) \approx 0.605651$ is the unique real root of the polynomial
 $\{96, -144, 86, -30, 9, -2\}$;
- $\varrho_2(\gamma^*) \approx 0.437941$ is the unique real root of the polynomial
 $\{7080, -8928, 6410, -2826, 621, -54\}$;
- $\varrho_3(\gamma^*) \approx 0.25655 + 0.54863i$ is the root of the polynomial
 $\{82944, -140544, 160624, -112944, 60516, -27800, 12636, -5832, 1969, -384, 36\}$
having the property $|\varrho_3(\gamma^*)| = \varrho_1(\gamma^*)$;
- $c_1(\gamma^*) \approx 1.21912$ is the unique real root of the polynomial
 $\{638976, -1308672, 767680, -148848, 255, -16\}$;
- $c_2(\gamma^*) \approx -0.583734$ is the unique real root of the polynomial
 $\{15582086307840, 11032756568064, 1374924543424, 141329286000,$
 $-715299903, 8503056\}$;
- $c_3(\gamma^*) \approx -0.123106 - 0.169757i$ is the root of the polynomial
 $\{654252399875063808, 147972616215330816, 117436085430648832,$
 $23378947275620352, 6522272391303168, 504776558675968, 75411131715456,$
 $-3364763918784, 58367021905, -452933856, 1679616\}$

having the smallest real part.

Remark 3.10. *Here again we have converted polynomials whose coefficients are algebraic numbers to higher-degree polynomials with integer coefficients (cf. Remark 3.7).*

By rewriting $\mu_n(\gamma^*)$ ($n \in \mathbb{N}$) as

$$(\varrho_1(\gamma^*))^n \left[c_1(\gamma^*) + c_2(\gamma^*) \left(\frac{\varrho_2(\gamma^*)}{\varrho_1(\gamma^*)} \right)^n + c_3(\gamma^*) \left(\frac{\varrho_3(\gamma^*)}{\varrho_1(\gamma^*)} \right)^n + \overline{c_3(\gamma^*)} \left(\frac{\overline{\varrho_3(\gamma^*)}}{\varrho_1(\gamma^*)} \right)^n \right],$$

and noticing that

$$\left| c_2(\gamma^*) \left(\frac{\varrho_2(\gamma^*)}{\varrho_1(\gamma^*)} \right)^n + c_3(\gamma^*) \left(\frac{\varrho_3(\gamma^*)}{\varrho_1(\gamma^*)} \right)^n + \overline{c_3(\gamma^*)} \left(\frac{\overline{\varrho_3(\gamma^*)}}{\varrho_1(\gamma^*)} \right)^n \right| \leq$$

$$|c_2(\gamma^*)| \left| \frac{\varrho_2(\gamma^*)}{\varrho_1(\gamma^*)} \right|^n + 2|c_3(\gamma^*)| \left| \frac{\varrho_3(\gamma^*)}{\varrho_1(\gamma^*)} \right|^n = |c_2(\gamma^*)| \left| \frac{\varrho_2(\gamma^*)}{\varrho_1(\gamma^*)} \right|^n + 2|c_3(\gamma^*)| <$$

$$|c_2(\gamma^*)| + 2|c_3(\gamma^*)| < 11/10 < |c_1(\gamma^*)|,$$

we see that $\mu_n(\gamma^*) > 0$ for all $n \in \mathbb{N}$. Thus we have proved $\gamma_{\text{sup},4} \geq \gamma^*$.

To prove the converse inequality, $\gamma_{\text{sup},4} \leq \gamma^*$, we apply Lemma 3.2. We set $\gamma := \gamma^* + \varepsilon$ with some sufficiently small, but arbitrary $\varepsilon > 0$. Then for $n \in \mathbb{N}$ we have

$$\mu_n(\gamma) = |\varrho_3(\gamma)|^n (\nu_n + wz^n + \bar{w}(\bar{z})^n)$$

with $z := \varrho_3(\gamma)/|\varrho_3(\gamma)|$, $w := c_3(\gamma)$ and

$$\nu_n := c_1(\gamma) \left(\frac{\varrho_1(\gamma)}{|\varrho_3(\gamma)|} \right)^n + c_2(\gamma) \left(\frac{\varrho_2(\gamma)}{|\varrho_3(\gamma)|} \right)^n.$$

Due to the properties of the numbers $\varrho_j(\gamma)$ listed in the paragraph of (21), we know that $\mathbb{R} \ni \nu_n \rightarrow 0$ as $n \rightarrow +\infty$. Moreover, since the functions $\varrho_3(\cdot)$ and $c_3(\cdot)$ are continuous (also) at γ^* , we have $z \in \mathbb{C} \setminus \mathbb{R}$, $|z| = 1$ and $w \in \mathbb{C} \setminus \{0\}$, for $\varepsilon > 0$ small enough. Lemma 3.2 then shows that $\mu_n(\gamma)$ cannot be non-negative for all $n \in \mathbb{N}$, so by Theorem 1.6 we obtain that $\gamma_{\text{sup},4} < \gamma^* + \varepsilon$.

3.5.5 The BDF5 method

The recursion (13) is

$$\begin{aligned} (60\gamma + 137)\mu_n(\gamma) - 300\mu_{n-1}(\gamma) + 300\mu_{n-2}(\gamma) - 200\mu_{n-3}(\gamma) + \\ 75\mu_{n-4}(\gamma) - 12\mu_{n-5}(\gamma) = 0 \quad (n \geq 5) \end{aligned}$$

with

$$\begin{aligned} \mu_0(\gamma) &= \frac{60}{60\gamma + 137}, \quad \mu_1(\gamma) = \frac{18000}{(60\gamma + 137)^2}, \quad \mu_2(\gamma) = \frac{18000(-60\gamma + 163)}{(60\gamma + 137)^3}, \\ \mu_3(\gamma) &= \frac{12000(3600\gamma^2 - 37560\gamma + 30469)}{(60\gamma + 137)^4}, \\ \mu_4(\gamma) &= \frac{4500(-216000\gamma^3 + 8600400\gamma^2 - 22146420\gamma + 10021847)}{(60\gamma + 137)^5}; \end{aligned}$$

see Figure 1.

The characteristic polynomial of the recursion $\mathcal{P}_5(\cdot, \gamma)$ has no multiple roots for $\gamma > 0$. We denote the five distinct roots of $\mathcal{P}_5(\cdot, \gamma)$ by $\varrho_{1,2,3,4,5}(\gamma)$ and let

$$\gamma^* \approx 0.30421$$

denote the 10th-degree algebraic number listed in the row of $\gamma_{\text{sup},5}$ in Theorem 2.3. Then for any $\gamma \in (0, 1)$ we can prove that

- $0 < \varrho_1(\gamma) < 1$ and $\varrho_{2,3,4,5}(\gamma) \in \mathbb{C} \setminus \mathbb{R}$;
- $|\varrho_{2,3,4,5}(\gamma)| < \varrho_1(\gamma)$ for $0 < \gamma < \gamma^*$;
- $|\varrho_{4,5}(\gamma^*)| < |\varrho_{2,3}(\gamma^*)| = \varrho_1(\gamma^*)$ for $\gamma = \gamma^*$;
- $|\varrho_{1,4,5}(\gamma)| < |\varrho_2(\gamma)| = |\varrho_3(\gamma)|$ for $\gamma^* < \gamma < 1$.

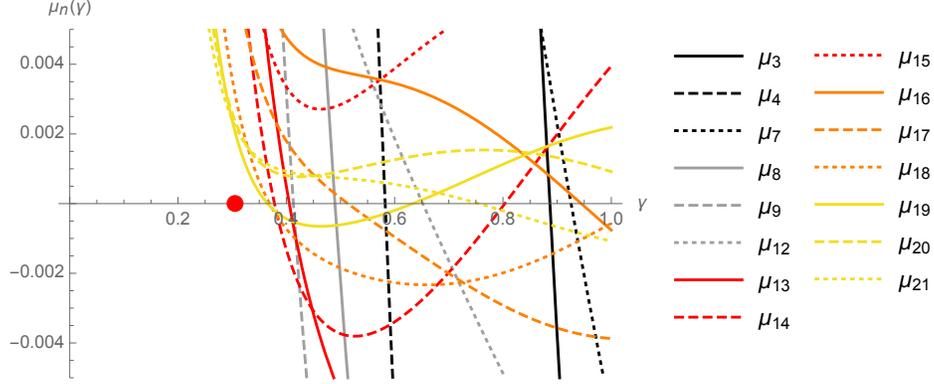


Figure 1: The functions $\gamma \mapsto \mu_n(\gamma)$ for $1 \leq n \leq 21$ corresponding to the BDF5 method are shown (the curves with indices $n \in \{1, 2, 5, 6, 10, 11\}$ are not visible in this plot window). The red dot is placed at $\gamma = \gamma_{\text{sup},5} \approx 0.30421$.

For $\gamma = \gamma^*$ and $n \geq 0$ we have

$$\mu_n(\gamma^*) = \varrho_1^n \left[c_1 + c_2 \left(\frac{\varrho_2}{\varrho_1} \right)^n + \bar{c}_2 \left(\frac{\bar{\varrho}_2}{\varrho_1} \right)^n + c_4 \left(\frac{\varrho_4}{\varrho_1} \right)^n + \bar{c}_4 \left(\frac{\bar{\varrho}_4}{\varrho_1} \right)^n \right],$$

where, for brevity, now we omit the explicit form of the algebraic numbers c_j and ϱ_j , and only give their approximate values:

- $\varrho_1 \approx 0.737893$, $\varrho_2 \approx 0.195442 + 0.711539i$, $\varrho_4 \approx 0.401777 + 0.175943i$,
- $c_1 \approx 0.994377$, $c_2 \approx -0.117157 - 0.126015i$, $c_4 \approx -0.186798 - 0.0841337i$.

From this we get that

$$\left| c_2 \left(\frac{\varrho_2}{\varrho_1} \right)^n + \bar{c}_2 \left(\frac{\bar{\varrho}_2}{\varrho_1} \right)^n + c_4 \left(\frac{\varrho_4}{\varrho_1} \right)^n + \bar{c}_4 \left(\frac{\bar{\varrho}_4}{\varrho_1} \right)^n \right| \leq 2|c_2| \cdot 1^n + 2|c_4| \cdot 1^n < \frac{8}{10} < c_1,$$

so $\mu_n(\gamma^*) > 0$ ($n \in \mathbb{N}$), and hence $\gamma_{\text{sup},5} \geq \gamma^*$ by (18).

The proof of the converse inequality, $\gamma_{\text{sup},5} \leq \gamma^*$, is again based on Lemma 3.2, and is completely analogous to the one presented in Section 3.5.4.

3.5.6 The BDF6 method

The recursion (13) is

$$\begin{aligned} 3(20\gamma + 49)\mu_n(\gamma) - 360\mu_{n-1}(\gamma) + 450\mu_{n-2}(\gamma) - 400\mu_{n-3}(\gamma) + 225\mu_{n-4}(\gamma) - \\ 72\mu_{n-5}(\gamma) + 10\mu_{n-6}(\gamma) = 0 \quad (n \geq 6) \end{aligned}$$

with

$$\mu_0(\gamma) = \frac{20}{20\gamma + 49}, \quad \mu_1(\gamma) = \frac{2400}{(20\gamma + 49)^2},$$

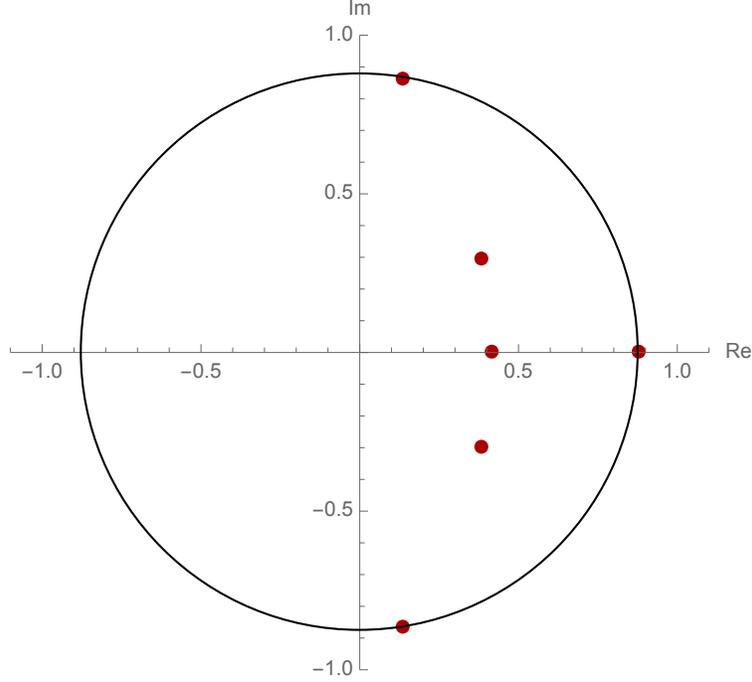


Figure 2: The roots of $\mathcal{P}_6(\cdot, \gamma_{\text{sup},6})$ corresponding to the BDF6 case.

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

Let us consider any $0 \leq \gamma < 37/60 \approx 0.6167$. Then one checks by using the discriminant that the 6 roots of $\mathcal{P}_6(\cdot, \gamma) = 0$ are distinct. Let

$$\gamma^* \approx 0.13136$$

denote the 18th-degree algebraic number listed in the row of $\gamma_{\text{sup},6}$ in Theorem 2.3. This constant has been obtained after some non-trivial computation and simplification. The roots $\varrho_j(\gamma)$ ($1 \leq j \leq 6$) are distributed as follows:

- $0 < \varrho_2(\gamma) < \varrho_1(\gamma) < 1$ and $\varrho_{3,4,5,6}(\gamma) \in \mathbb{C} \setminus \mathbb{R}$;
- $|\varrho_{2,3,4,5,6}(\gamma)| < \varrho_1(\gamma)$ for $0 < \gamma < \gamma^*$;
- $|\varrho_{2,5,6}(\gamma^*)| < |\varrho_{3,4}(\gamma^*)| = \varrho_1(\gamma^*)$ for $\gamma = \gamma^*$;
- $|\varrho_{1,2,5,6}(\gamma)| < |\varrho_3(\gamma)| = |\varrho_4(\gamma)|$ for $\gamma^* < \gamma < 37/60$.

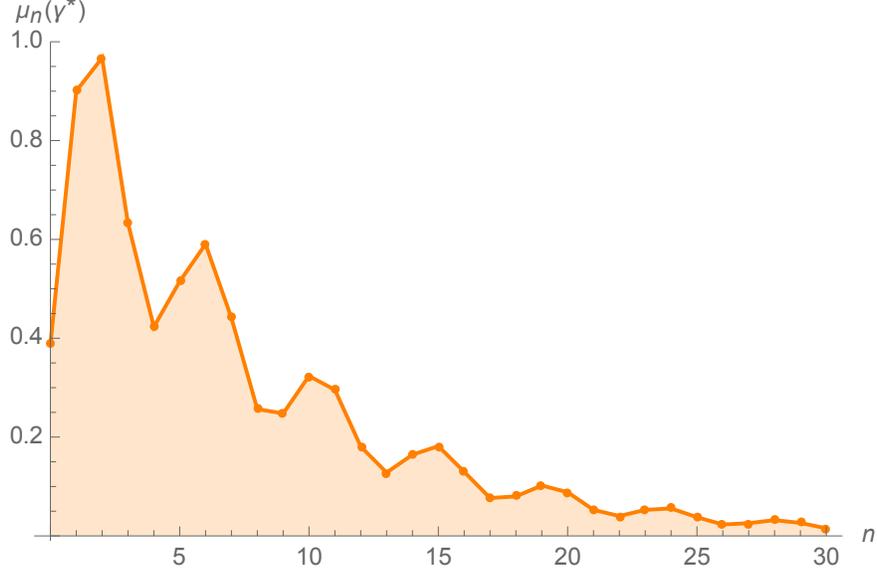


Figure 3: The sequence $\mu_n(\gamma^*)$ corresponding to the BDF6 method is depicted (using linear interpolation).

For $\gamma = \gamma^*$ and $n \geq 0$, one has the representation

$$\mu_n(\gamma^*) = \varrho_1^n \left[c_1 + c_2 \left(\frac{\varrho_2}{\varrho_1} \right)^n + c_3 \left(\frac{\varrho_3}{\varrho_1} \right)^n + \bar{c}_3 \left(\frac{\bar{\varrho}_3}{\varrho_1} \right)^n + c_5 \left(\frac{\varrho_5}{\varrho_1} \right)^n + \bar{c}_5 \left(\frac{\bar{\varrho}_5}{\varrho_1} \right)^n \right],$$

where the algebraic numbers c_j, ϱ_j have the approximate values

- $\varrho_1 \approx 0.87690236, \quad \varrho_2 \approx 0.41284041,$
- $\varrho_3 \approx 0.13673253 + 0.86617664i, \quad \varrho_5 \approx 0.38057439 + 0.29512217i,$
- $c_1 \approx 1.0000077, \quad c_2 \approx -0.13742979,$
- $c_3 \approx -0.11295491 - 0.10160183i, \quad c_5 \approx -0.124637633 - 0.050848744i,$

see Figure 2. For any $n \geq 0$, the estimate

$$\left| c_2 \left(\frac{\varrho_2}{\varrho_1} \right)^n + c_3 \left(\frac{\varrho_3}{\varrho_1} \right)^n + \bar{c}_3 \left(\frac{\bar{\varrho}_3}{\varrho_1} \right)^n + c_5 \left(\frac{\varrho_5}{\varrho_1} \right)^n + \bar{c}_5 \left(\frac{\bar{\varrho}_5}{\varrho_1} \right)^n \right| \leq$$

$$|c_2| + 2|c_3| + 2|c_5| < \frac{8}{10} < c_1$$

yields $\mu_n(\gamma^*) > 0$, see Figure 3. This proves that $\gamma_{\text{sup},6} \geq \gamma^*$ by (18).

As before, a final application of Lemma 3.2 shows that $\gamma_{\text{sup},6} \leq \gamma^*$, completing the proof.

3.6 Proofs for the Adams–Bashforth methods

The coefficients for the Adams–Bashforth methods are listed, for example, in [3].

3.6.1 The AB1 method

It is easily seen that the recursion (7) now has the form

$$\mu_n(\gamma) = (1 - \gamma)\mu_{n-1}(\gamma) \quad (n \geq 2)$$

with $\mu_1(\gamma) = 1$, so any $\gamma > 1$ violates the non-negativity of $\mu_n(\gamma)$ in (8). Hence $\gamma_{\text{sup},1} \leq 1$. But $\mu_n(1) \geq 0$ for all $n \in \mathbb{N}$, and it is known [4] that $-1 \in \text{int}(\mathcal{S})$, so (19) finishes the proof.

3.6.2 The AB2 method

For this method, the recursion (7) is

$$\mu_n(\gamma) - \left(1 - \frac{3\gamma}{2}\right)\mu_{n-1}(\gamma) - \frac{\gamma}{2}\mu_{n-2}(\gamma) = 0 \quad (n \geq 3)$$

with $\mu_1(\gamma) = 3/2$ and $\mu_2(\gamma) = -9\gamma/4 + 1$. Lemma 3.1 with $n = 2$ and $\gamma^* = 4/9$ shows that $\gamma_{\text{sup},2} \leq 4/9$. On the other hand,

$$\mu_n(4/9) = 3^{1-n} (2^n - 4(-1)^n) / 4 \geq 0 \quad (n \geq 1),$$

and $-4/9 \in \text{int}(\mathcal{S})$ (see [4]), so the proof is complete due to (19).

3.6.3 The AB3 method

For this method, the recursion (7) takes the form

$$\mu_n(\gamma) - \left(1 - \frac{23\gamma}{12}\right)\mu_{n-1}(\gamma) - \frac{4}{3}\gamma\mu_{n-2}(\gamma) + \frac{5}{12}\gamma\mu_{n-3}(\gamma) = 0 \quad (n \geq 4)$$

with

$$\mu_1(\gamma) = \frac{23}{12}, \quad \mu_2(\gamma) = -\frac{529\gamma}{144} + \frac{7}{12}, \quad \mu_3(\gamma) = \frac{12167\gamma^2}{1728} - \frac{161\gamma}{72} + 1.$$

Lemma 3.1 with $n = 2$ and $\gamma^* = 84/529$ shows that $\gamma_{\text{sup},3} \leq 84/529$. We also know [4] that $-84/529 \in \text{int}(\mathcal{S})$, so by (19) it is enough to verify that $\mu_n(84/529) \geq 0$ for all $n \geq 1$.

For $n \geq 1$ we have

$$\mu_n(84/529) = \sum_{j=1}^3 c_j \varrho_j^n = \varrho_3^n \left(c_3 + c_1 \left(\frac{\varrho_1}{\varrho_3}\right)^n + c_2 \left(\frac{\varrho_2}{\varrho_3}\right)^n \right),$$

where the numbers ϱ_j ($\varrho_1 < 0 < \varrho_2 < \varrho_3$, $|\varrho_1| < \varrho_3/2$, $\varrho_2 < \varrho_3/4$) and c_j ($-5 < c_1 < -3 < c_2 < 0 < 1 < c_3$) are the three roots of the polynomials $\{529, -368, -112, 35\}$ and

$$\{30733417008, 193547352348, 162435667337, -391554926405\},$$

respectively. Since

$$\left| c_1 \left(\frac{\varrho_1}{\varrho_3}\right)^n + c_2 \left(\frac{\varrho_2}{\varrho_3}\right)^n \right| \leq 5 \left| \frac{\varrho_1}{\varrho_3} \right|^n + 3 \left| \frac{\varrho_2}{\varrho_3} \right|^n < \frac{5}{2^n} + \frac{3}{4^n} < 1 < c_3$$

for $n \geq 3$, and $\mu_n(84/529) \geq 0$ for $1 \leq n \leq 2$, the proof is complete.

3.6.4 The AB4 method

The starting terms of the recursion (7) satisfy

$$\mu_1(\gamma) = \frac{55}{24}, \quad \mu_2(\gamma) = -\frac{3025\gamma}{576} - \frac{1}{6},$$

so the non-negativity condition in (8) for $n = 2$ is violated for any $\gamma > 0$, hence \nexists SCB > 0 .

4 Conclusions

The step-size coefficient for boundedness (SCB) of a linear multistep method (LMM) is a generalization of the strong-stability-preserving (SSP) coefficient of the LMM. The SCB appears in conditions that ensure monotonicity or boundedness properties of the LMM, and a method is more efficient if it possesses a larger SCB.

In [9, 16], a necessary and sufficient condition has been given for a number $\gamma > 0$ to be a SCB of a LMM. This condition involves checking the non-negativity of an auxiliary sequence $\mu_n(\gamma)$ that satisfies a linear recurrence relation in $n \in \mathbb{N}$. For fixed n , the function $\mu_n(\cdot)$ is a rational function.

The main goal of the present work is to determine the maximum SCB, γ_{sup} for a given linear multistep method. For each k -step BDF method ($2 \leq k \leq 6$) and each k -step Adams–Bashforth method ($1 \leq k \leq 3$), we determine the exact value of γ_{sup} by finding the largest $\gamma > 0$ that satisfies $\mu_n(\gamma) \geq 0$ for all non-negative n .

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 $\gamma = \gamma_{\text{sup}}$, 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.

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