Existence and optimality of strong stability preserving linear multistep methods: a duality-based approach

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Abstract

We prove the existence of explicit linear multistep methods of any order with positive coefficients. Our approach is based on formulating a linear programming problem and establishing infeasibility of the dual problem. This yields a number of other theoretical advances.

1 Introduction

In this work we study numerical methods for the solution of the initial value problem (IVP)

\[ u'(t) = f(t, u) \quad u(t_0) = u_0 \quad t_0 \leq t \leq T, \]

under the assumption that the solution is monotone in time:

\[ \|u(t + h)\| \leq \|u(t)\| \quad \forall h \geq 0. \]

Here \( u : \mathbb{R} \rightarrow \mathbb{R}^m \), and \( \| \cdot \| \) is any convex functional. The theory pursued herein is also relevant when \( u \) satisfies a contractivity or positivity condition. We will usually write \( f(u) \) instead of \( f(t, u) \) merely to keep the notation simpler.

We focus on the class of methods for solving (1) that are known as linear multistep methods (LMMs). To solve (1) by a linear multistep method, we define a sequence of times \( t_0 < t_1 < \ldots < t_N = T \) where \( t_n := t_{n-1} + h \), and compute the values \( u_n \approx u(t_n) \) sequentially by

\[ u_n = \sum_{j=0}^{k-1} a_j u_{n-k+j} + h \sum_{j=0}^{k} b_j f(u_{n-k+j}). \]

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Some prescription must be given for the starting values $u_0, \ldots, u_{k-1}$. If $\beta_k = 0$, the method is said to be explicit; otherwise it is implicit.

We are interested in methods that preserve a discrete version of the monotonicity condition (2); namely

$$\|u_n\| \leq \max \{ \|u_{n-1}\|, \ldots, \|u_{n-k}\| \}. \quad (4)$$

The backward Euler method achieves (4) under any step size, as long as $f$ is such that (2) is satisfied.

In order to achieve the discrete monotonicity property (4) with explicit methods, or with implicit methods of higher order, we assume a stronger condition than (2). We require that $f$ be monotone under a forward Euler step, with some restriction on the step size:

$$\|u + hf(u)\| \leq \|u\| \quad \forall 0 \leq h \leq h_{FE}(u). \quad (5)$$

Under assumption (5) it can be shown that any method (3) with non-negative coefficients preserves discrete monotonicity (4) under some time step restriction. The maximum step size that guarantees monotonicity is

$$Ch_{FE}. \quad (6)$$

where

$$C = \min_{j : \beta_j \neq 0} \frac{\alpha_j}{\beta_j} \quad (7)$$

is known as the threshold factor or strong stability preserving coefficient (SSP coefficient) of the method. If a method has any negative coefficient, we say $C = 0$.

Runge–Kutta methods with positive SSP coefficient are subject to restrictive order barriers: explicit methods have order at most four and implicit methods have order at most six. SSP linear multistep methods of high order are therefore of particular interest. The objective of the present work is to investigate existence of methods with $C > 0$ and bounds on the value of $C$ for methods with a prescribed order of accuracy and number of steps.

In this paper we have assumed a fixed step size; the case of SSP explicit linear multistep methods with variable step size is covered in [HKLN].

1.1 Previous work

Contractive linear multistep methods were studied by Sand, who constructed a family of implicit methods with arbitrarily high order [San86, Theorem 2.3] whose number of steps is exponential in the order of accuracy. Later Lenferink deduced many properties of the optimal methods and threshold factors for low order methods [Len89, Len91]. More recently, such methods have been studied by Hundsdorfer & Ruuth [HR05, RH05], who consider the effect of special starting procedures and of requiring only boundedness rather than strict contractivity or monotonicity. A fast algorithm for computing optimal methods, along with extensive results, was given in [Ket09].
1.2 Scope and main results

Linear multistep methods are closely related to polynomial interpolation formulas. We investigate their properties herein using the framework of linear programming and results on polynomial interpolants.

The main results proved in the present work are:

1. Existence of arbitrary order explicit LMMs with $C > 0$;
2. A sharper upper bound on $C$ for implicit LMMs;
3. Behavior of the optimal value of $C$ for $k$-step methods as $k \to \infty$.

Along the way, we also give a new proof of the known upper bound on $C$ for explicit LMMs, and a new relation between $C$ for certain implicit and explicit classes of LMMs.

2 Formulation as a linear programming feasibility problem

By replacing $u_n$ with the exact solution $u(t_n)$ in (3) and expanding terms in Taylor series about $t_{n-k}$, we obtain the following conditions for method (3) to be consistent of order $p$:

\[
\sum_{j=0}^{k-1} \alpha_j = 1 \quad (8a)
\]

\[
\sum_{j=0}^{k-1} \left( j^m \alpha_j + mj^{m-1} \beta_j \right) + mk^{m-1} \beta_k = k^m \quad 1 \leq m \leq p; \quad (8b)
\]

A linear multistep method (3) has SSP coefficient at least equal to $r > 0$ iff

\[
\beta_k \geq 0 \quad \text{and} \quad \beta_j \geq 0 \quad \alpha_j - r \beta_j \geq 0 \quad \text{for all } 0 \leq j \leq k - 1.
\]

Thus the problem of whether there exists a method of order $p$ with $k$ steps and SSP coefficient at least $r > 0$ can be formulated for explicit methods as [Ket09, LP 2]:

\[
\begin{align*}
\text{Find} & \quad \beta_j \geq 0 \quad \delta_j \geq 0 & \text{for } 0 \leq j \leq k - 1 \\
\text{such that} & \quad \sum_{j=0}^{k-1} \left( (\delta_j + r \beta_j) j^i + \beta_j i j^{i-1} \right) = k^i & \text{for } 0 \leq i \leq p,
\end{align*}
\]
and for implicit methods as:

\[ \text{Find} \]
\[ \beta_k \geq 0 \quad \text{and} \quad \beta_j \geq 0 \quad \delta_j \geq 0 \quad \text{for } 0 \leq j \leq k - 1 \]
such that
\[ \sum_{j=0}^{k-1} \left( (\delta_j + r\beta_j) j^i + \beta_j j^{i-1} \right) + \beta_k i^{i-1} = k^i \quad \text{for } 0 \leq i \leq p. \]

In both cases, \( a_j \) can be obtained for a fixed \( r \) via 
\[ a_j = \delta_j + r\beta_j \quad \text{for all } 1 \leq j \leq k - 1. \]

3 Optimality conditions for SSP methods

In this section we develop the basic tools used in this paper. Our analysis relies on Farkas’ lemma and on the Duality and Complementary slackness theorems in linear programming (LP), which we now recall; see, e.g. \[ \text{Sch98} \].

**Proposition 3.1** (Farkas’ lemma). Let \( A \in \mathbb{R}^{m \times n} \) be a matrix and let \( b \in \mathbb{R}^m \) be a vector. The system \( Ax = b, x \geq 0 \) is feasible if and only if the system \( A^\top y \geq 0, b^\top y < 0 \) is infeasible.

**Proposition 3.2** (Duality theorem in linear programming). Let \( A \in \mathbb{R}^{m \times n} \) be a matrix and let \( b \in \mathbb{R}^m, c \in \mathbb{R}^n \) be vectors. Consider the primal-dual pair of LP problems

Maximize \( c^\top x \) subject to \( Ax = b \) and \( x \geq 0 \), (11a)

Minimize \( b^\top y \) subject to \( A^\top y \geq c \). (11b)

If both problems are feasible, then the two optima are equal.

**Proposition 3.3** (Complementary slackness theorem). Let \( A \in \mathbb{R}^{m \times n} \) be a matrix and let \( b \in \mathbb{R}^m, c \in \mathbb{R}^n \) be vectors. Consider the primal-dual pair of LP problems (11). Assume that both optima are finite, let \( x_0 \) be an optimal solution to (11a) and let \( y_0 \) be an optimal solution to (11b). Then \( x_0^\top (b - A^\top y_0) = 0 \), i.e. if a component of \( x_0 \) is positive, then the corresponding inequality in \( A^\top y \geq c \) is satisfied by \( y_0 \) with equality.

The following two lemmas are simple consequences of Farkas’ lemma.

**Lemma 3.1.** Let \( r \in \mathbb{R} \) be arbitrary and let \( k, p \) be positive integers. The following statements are equivalent:

(i) The LP feasibility problem (9) is infeasible.
(ii) There exist \( y_i \in \mathbb{R} \) for \( 0 \leq i \leq p \) that satisfy the system

\[
\begin{align*}
\sum_{m=0}^{p} j^m y_m & \geq 0 & \text{for } 0 \leq j \leq k - 1 \\
\sum_{m=0}^{p} \left( m j^{m-1} y_m + r j^m y_m \right) & \geq 0 & \text{for } 0 \leq j \leq k - 1 \\
\sum_{m=0}^{p} k^m y_m & < 0.
\end{align*}
\]

(iii) There exists a real univariate polynomial \( q \) of degree at most \( p \) that satisfies the conditions

\[
\begin{align*}
q(j) & \geq 0 & \text{for } 1 \leq j \leq k \\
-q'(j) + r \cdot q(j) & \geq 0 & \text{for } 1 \leq j \leq k \\
q(0) & < 0.
\end{align*}
\]

Proof. **Step 1.** Since (12) is the Farkas dual of (9), the equivalence of (i) and (ii) is a direct consequence of Proposition 3.1.

**Step 2.** We show the equivalence of (ii) and (iii). Suppose that \( y_i \) for \( i = 1, \ldots, p \) satisfy conditions (12). Then \( q(x) := \sum_{m=0}^{p} y_m (k-x)^m \) is a real univariate polynomial of degree at most \( p \). This \( q \) satisfies condition (13c) because of (12c), and satisfies conditions (13a) and (13b) for any \( 1 \leq j_0 \leq k \), due to (12a) and (12b) for index \( j = k - j_0 \).

Now suppose that \( q \) is a real univariate polynomial of degree at most \( p \) that satisfies conditions (13). Define \( y_m := (-1)^m \cdot q^{(m)}(k) \) for \( m = 1, \ldots, p \). Then the values \( y_m \) are real, and \( q(x) = \sum_{m=0}^{p} y_m (k-x)^m \) just as before. Therefore conditions (12) are satisfied by \( y_m \) for \( m = 1, \ldots, p \), as a consequence of conditions (13). \( \square \)

**Lemma 3.2.** Let \( r \in \mathbb{R} \) and let \( k, p \) be positive integers. The following statements are equivalent:

(i) The LP feasibility problem (10) is infeasible.

(ii) There exist \( y_i \in \mathbb{R} \) for \( 0 \leq i \leq p \) that satisfy the system defined by (12a)–(12c) and

\[
\sum_{m=0}^{p} m k^{m-1} y_m \geq 0.
\]

(iii) There exists a real univariate polynomial \( q \) of degree at most \( p \) that satisfies (13a)–(13c) and

\[
-q'(0) \geq 0.
\]

Proof. The proof is essentially the same as in Lemma 3.1 \( \square \)
We present three auxiliary lemmas that will be used in the proofs of Lemmas 3.6–3.9. From now on by polynomial we mean a real polynomial in one variable.

**Lemma 3.3.** Let \( r \in \mathbb{R} \) and let \( k \) be a positive integer, and let \( q \) be a non-zero polynomial of degree \( p_0 > 0 \). In view of the Fundamental theorem of algebra and the Conjugate root theorem, this polynomial can be uniquely written in the form \( q(x) = c \cdot \prod_{m=1}^{p_0} (x - \lambda_m) \), where \( c \in \mathbb{R} \setminus \{0\} \) is the leading coefficient of the polynomial and \( \lambda_1, \lambda_2, \ldots, \lambda_{p_0} \in \mathbb{C} \) are the roots of the polynomial, moreover non-real roots occur in conjugate pairs. Let us introduce the notation \( n(j) := |\{m : 1 \leq m \leq p_0, \text{Re}\lambda_m \geq j\}| \). Then the following statements hold.

(i) Condition \((13a)\) is satisfied by \( q \) if and only if for all \( 1 \leq j \leq k \): either \( j \) is a root of \( q \), or

\[ c \cdot (-1)^{n(j)} > 0. \]  \hspace{1cm} (16a)

(ii) Suppose that condition \((13a)\) is satisfied by \( q \). Then \( q \) satisfies \((13b)\) if and only if for all \( 1 \leq j \leq k \):
- either \( j \) is a multiple root of \( q \), or \( j \) is a root of \( q \) and \((16a)\) holds for index \( j \), or \( j \) is not a root of \( q \) and

\[ \sum_{m=1}^{p_0} \frac{1}{j - \lambda_m} \leq r. \]  \hspace{1cm} (16b)

(iii) Condition \((13c)\) is satisfied by \( q \) if and only if \( 0 \) is not a root of \( q \) and

\[ c \cdot (-1)^{n(0)} < 0. \]  \hspace{1cm} (16c)

(iv) Suppose that condition \((13c)\) is satisfied by \( q \). Then \( q \) satisfies \((15)\) if and only if

\[ \sum_{m=1}^{p_0} \frac{1}{\lambda_m} \leq 0. \]  \hspace{1cm} (16d)

**Proof.** The proof of the lemma can be easily deduced using the above expression for \( q \), and the expression \( \frac{q(j)}{q'(j)} = \sum_{m=1}^{p_0} \frac{1}{j - \lambda_m} \) for the logarithmic derivative of the polynomial. \( \square \)

**Lemma 3.4.** Let \( r \in \mathbb{R} \) and let \( k, p \) be positive integers. Suppose that a polynomial \( q \) of degree \( 0 < p_0 \leq p \) satisfies conditions \((13a)\)–\((13c)\). Then there exists a polynomial \( \tilde{q} \) of degree \( p \) that satisfies conditions \((13a)\) and \((13b)\), has a leading coefficient \( \pm 1 \), furthermore its roots \( \tilde{\lambda}_1, \tilde{\lambda}_2, \ldots, \tilde{\lambda}_p \) satisfy the following conditions.

\[ \tilde{\lambda}_m \in \mathcal{H} := \{z \in \mathbb{C} : |\text{Im}(z)| \leq (k - 1)/2, 0 \leq \text{Re}(z) \leq k \} \quad \text{for } 1 \leq m \leq p \]  \hspace{1cm} (17a)

\[ 0 \text{ is a simple root of } \tilde{q}. \]  \hspace{1cm} (17b)
Proof. Suppose that the assumptions made in the lemma hold for some polynomial \( q \). Then the polynomial \( q + |q(0)|/2 \) has the same degree as \( q \), all of its roots are in \( C \setminus \{0, 1, \ldots, k\} \), moreover it satisfies the same conditions as \( q \). Hence \( q(j) > 0 \) for all \( 1 \leq j \leq k \). Therefore, in view of Lemma 3.3, \( q(x) = c \cdot \prod_{m=1}^{p_0} (x - \lambda_m) \), where \( c \in \mathbb{R} \setminus \{0\} \) and \( \lambda_1, \lambda_2, \ldots, \lambda_{p_0} \in C \setminus \{0, 1, \ldots, k\} \); furthermore the non-real roots occur in conjugate pairs and inequalities \( (16a) - (16c) \) hold for all \( 1 \leq j \leq k \).

Because of inequalities \( (16c) \) and \( (16a) \) for index \( j = 1 \), and because non-real roots occur in conjugate pairs, there exists an index \( 1 \leq k \leq p \) such that \( \lambda_{m_0} \in (0, 1) \). Let us define the sets \( \mathcal{M} := \{ l : 0 \leq l \leq p_0, \lambda_l \notin \mathcal{H} \} \) and \( \mathcal{M}_0 := \{ l : 0 \leq l \leq p_0, \lambda_l \notin \mathcal{H}, \text{Re}(\lambda_l) < k \} \). We set

\[
\tilde{c} := (-1)^{\mathcal{M}_0} \cdot c \cdot \prod_{m=1}^{p} (x - \bar{\lambda}_m).
\]

One easily checks that \( \tilde{q} \) is a real polynomial of degree \( p \), that its leading coefficient \( \tilde{c} \) is either 1 or \(-1\), and that conditions \( (17a) - (17b) \) hold. Due to their construction, \( \tilde{\lambda}_1, \tilde{\lambda}_2, \ldots, \tilde{\lambda}_p \) satisfy inequality \( (16a) \) for all \( 1 \leq j \leq k \), since the same conditions are satisfied by \( \lambda_1, \lambda_2, \ldots, \lambda_{p_0} \), and \( \tilde{c} \cdot (-1) \) for all \( 1 \leq j \leq k \). Therefore, due to statement (i) of Lemma 3.3, condition \( (13a) \) is satisfied by \( \tilde{q} \).

Now we show that condition \( (13b) \) is satisfied by \( \tilde{q} \).

Case \( \mathcal{M} + p - p_0 = 0 \): No new roots were introduced, and \( \lambda_{m_0} \) is the only root that was moved. Replacing \( \lambda_{m_0} \) with 0 clearly decreases the left-hand-side of \( (16b) \), hence \( (16b) \) is also satisfied by \( \tilde{\lambda}_1, \tilde{\lambda}_2, \ldots, \tilde{\lambda}_p \) for all \( 1 \leq j \leq k \). Therefore, in view of statement (ii) of Lemma 3.3, condition \( (13b) \) is satisfied by \( \tilde{q} \).

Case \( \mathcal{M} + p - p_0 > 0 \): Since \( k \) is a root of \( \tilde{q} \), and since inequality \( (16a) \) holds for index \( j = k \), the conditions of statement (ii) of Lemma 3.3 are met for \( j = k \). Replacing \( \lambda_{m_0} \) with 0 and replacing the roots with a negative real part by \( k \), and replacing larger than \( k \) real roots with \( k \) clearly decreases the left-hand-side of \( (16b) \) for all \( 1 \leq j \leq k - 1 \).

The contribution of \( \lambda \) and \( \bar{\lambda} \), a pair of conjugate roots with \( \text{Im}(\lambda) > (k - 1)/2 \), to the left-hand-side of \( (16b) \) is \( \frac{1}{j - \lambda} + \frac{1}{j - \bar{\lambda}} = \frac{2(j - \text{Re}(\lambda))}{(j - \text{Re}(\lambda))^2 + (\text{Im}(\lambda))^2} \geq \frac{1}{(j - \text{Re}(\lambda))^2 + (\text{Im}(\lambda))^2} \geq \frac{2}{j - k} \) for all \( 1 \leq j \leq k - 1 \), therefore replacing such roots with \( k \) decreases the left-hand-side of \( (16b) \).

The contribution of \( \lambda \) and \( \bar{\lambda} \), a pair of conjugate roots with \( \text{Re}(\lambda) > k \), to the left-hand-side of \( (16b) \) is \( \frac{1}{j - \lambda} + \frac{1}{j - \bar{\lambda}} = \frac{2(i - \text{Re}(\lambda))}{(i - \text{Re}(\lambda))^2 + (\text{Im}(\lambda))^2} \geq \frac{2}{\text{Re}(\lambda) - j} \) for all \( 1 \leq j \leq k - 1 \), therefore replacing such roots with \( k \) decreases the left-hand-side of \( (16b) \).

Thus the inequality \( (16b) \) is also satisfied by \( \lambda_1, \lambda_2, \ldots, \lambda_p \) for all \( 1 \leq j \leq k - 1 \). Therefore, in view of statement (ii) of Lemma 3.3, the condition \( (13b) \) is satisfied by \( \tilde{q} \).
Lemma 3.5. Let \( r \in \mathbb{R} \) and let \( k, p \) be positive integers. Suppose that a polynomial \( q \) of degree \( 0 < p_0 \leq p \) satisfies conditions (13a)–(13c) and condition (15). Then there exist a polynomial \( \tilde{q} \) of degree \( p \) that satisfies conditions (13a) and (13b), has a leading coefficient \( \pm 1 \), and its roots \( \hat{\lambda}_1, \hat{\lambda}_2, \ldots, \hat{\lambda}_p \) satisfy the condition (17a), furthermore

\[
0 \text{ is a root of } \tilde{q} \text{ with multiplicity } 2.
\]  

Proof. Suppose that the assumptions made in the lemma hold for some polynomial \( q \). As in Lemma 3.4 we can safely assume that \( q(x) = c \cdot \prod_{m=1}^{p_0}(x - \lambda_m) \), where \( c \in \mathbb{R} \setminus \{0\} \) and \( \lambda_1, \lambda_2, \ldots, \lambda_{p_0} \in \mathbb{C} \setminus \{0, 1, \ldots, k\} \), that the non-real roots occur in conjugate pairs, furthermore that inequalities (16a)–(16d) hold for all \( 1 \leq j \leq k \).

First we show that we can transform \( q \) in a few steps into a polynomial \( \tilde{q} \) of degree \( 0 \leq \tilde{p} \leq p_0 \) that meets the conditions of the lemma, and has exactly one (necessarily real) root with a negative real part.

**Step 1.** Let us define the set \( \mathcal{M}_1 := \{ m : 1 \leq m \leq p_0, \text{Re}(\lambda_m) < 0 \} \). We set

\[
\hat{\lambda}_{m,0} := \begin{cases} 
\frac{\lambda_m}{(\text{Re}(\lambda_m))^2 + (\text{Im}(\lambda_m))^2} & \text{if } 1 \leq m \leq p_0 \text{ and } m \not\in \mathcal{M}_1 \\
\frac{\lambda_m}{\text{Re}(\lambda_m)} & \text{if } 1 \leq m \leq p_0 \text{ and } m \in \mathcal{M}_1
\end{cases}
\]

\[
\hat{q}_0(x) := c \cdot \prod_{m=1}^{p_0} (x - \hat{\lambda}_{m,0}).
\]

One easily checks that \( \hat{q}_0 \) is a real polynomial of degree \( p_0 \), and that its roots \( \hat{\lambda}_{1,0}, \hat{\lambda}_{2,0}, \ldots, \hat{\lambda}_{p_0,0} \) satisfy inequalities (16a) and (16c)–(16d). The contribution of \( \lambda \) and \( \overline{\lambda} \), a pair of conjugate roots with \( \text{Re}(\lambda) < 0 \), to the left-hand-side of (16b) is

\[
\frac{2}{j^+ |\text{Re}(\lambda)| + (\text{Re}(\lambda))^2/|\text{Re}(\lambda)|^2} \geq \frac{2}{j^- |\text{Re}(\lambda)| + (\text{Re}(\lambda))^2/|\text{Re}(\lambda)|^2} \geq \frac{2}{j^- |\text{Re}(\lambda)| + (\text{Re}(\lambda))^2/|\text{Re}(\lambda)|^2} \geq \frac{2}{j^- |\text{Re}(\lambda)| + (\text{Re}(\lambda))^2/|\text{Re}(\lambda)|^2}
\]

for all \( 1 \leq j \leq k \), hence replacing such roots with \( \frac{\text{Re}(\lambda)}{\text{Re}(\lambda)} \) decreases the left-hand-side of (16b), therefore \( \hat{\lambda}_{1,0}, \hat{\lambda}_{2,0}, \ldots, \hat{\lambda}_{p_0,0} \) also satisfy inequality (16b) for all \( 1 \leq j \leq k \). Let us set \( l := 0 \).

**Step 2.** Let us consider \( \hat{\lambda}_{1,l}, \hat{\lambda}_{2,l}, \ldots, \hat{\lambda}_{p_l,l} \) that we defined earlier. As a result of previous steps, \( \hat{\lambda}_{1,l}, \hat{\lambda}_{2,l}, \ldots, \hat{\lambda}_{p_l,l} \) satisfy inequalities (16a)–(16d), and all of them with a negative real part are real. Suppose that \( \hat{\lambda}_{m_1,l}, \hat{\lambda}_{m_2,l} < 0 \) for some indices \( 0 \leq m_1 < m_2 < p_l \). Let us set

\[
p_{l+1} := p_l - 1
\]

\[
\hat{\lambda}_{m,l+1} := \begin{cases} 
\frac{\hat{\lambda}_{m,l}}{1/\hat{\lambda}_{m_1,l} + 1/\hat{\lambda}_{m_2,l}} & \text{if } 1 \leq m \leq m_1 \text{ or } m_1 < m < m_2 \\
\hat{\lambda}_{m_{l-1},l} & \text{if } m = m_1 \\
\hat{\lambda}_{m_{l-1},l} & \text{if } m_2 \leq m \leq p_{l+1}
\end{cases}
\]

\[
\hat{q}_{l+1}(x) := c \cdot \prod_{m=1}^{p_{l+1}} (x - \hat{\lambda}_{m,l+1}).
\]

In both cases, the proof of the lemma is complete. \( \square \)
One easily checks that \(\hat{q}_{l+1}\) is a real polynomial of degree \(p_{l+1}\), and that \(\hat{\lambda}_{1,l+1}, \hat{\lambda}_{2,l+1}, \ldots, \hat{\lambda}_{p_{l+1},l+1}\) satisfy inequalities (16a) and (16c)–(16d). The contribution of \(\lambda := \hat{\lambda}_{m_1,l} < 0\) and \(\tilde{\lambda} := \hat{\lambda}_{m_2,l} < 0\) to the left-hand-side of (16b) is \(\frac{1}{j-\lambda} + \frac{1}{j-\hat{\lambda}} = \frac{2}{j-\lambda} - \frac{\lambda/p}{j-\lambda} \geq \frac{1}{j-\lambda} - \frac{1}{j-\hat{\lambda}}\) for all \(1 \leq j \leq k\), since we can rearrange the inequality into \(j(\lambda + \hat{\lambda} - \lambda) \geq 0\), and that holds for all \(1 \leq j \leq k\). Hence replacing the pair of roots \(\frac{\lambda_{m_1,l} \cdot \lambda_{m_2,l}}{\lambda_{m_1,l} + \lambda_{m_2,l}}\) decreases the left-hand-side of (16b), therefore \(\hat{\lambda}_{1,l+1}, \hat{\lambda}_{2,l+1}, \ldots, \hat{\lambda}_{p_{l+1},l+1}\) also satisfy inequality (16b) for all \(1 \leq j \leq k\).

**Step 3.** We set \(l := l + 1\) and repeat Step 2 until \(\hat{q}_l\) has only one negative real root. Then \(\tilde{q} := \hat{q}_l\) is a real polynomial of degree \(\hat{p} := p_l\) that satisfies conditions (13a)–(13c) and (15), due to statements (i)–(iv) of Lemma 3.3, furthermore it has only one root with a negative real part, and this root is real. The proof of this claim is complete.

The latter property of \(\tilde{q}\), together with inequalities (16c) and (16a) for index \(j = 1\), imply that \(\hat{\lambda}_{m_0} \in (0,1)\) and \(\hat{\lambda}_{m_1} < 0\) for some indices \(1 \leq m_0, m_1 \leq \hat{p}\). Let us recall the definitions of \(\mathcal{M}\) and \(\mathcal{M}_0\) given in Lemma 3.4 and let us set

\[
\bar{c} := (-1)^{\lfloor \mathcal{M}_0 \rfloor - 1 + \hat{p} - \hat{p}} \frac{C}{|C|}
\]

\[
\bar{\lambda}_m := \begin{cases} 
\hat{\lambda}_m & \text{if } 1 \leq m \neq m_0 \leq \hat{p} \text{ and } m \notin \mathcal{M} \\
0 & \text{if } m = m_0 \text{ or } m = m_1 \\
k & \text{if } \hat{p} < m \leq p, \text{ or if } m \neq m_1 \text{ and } m \in \mathcal{M}
\end{cases}
\]

\[
\bar{q}(x) := \bar{c} \cdot \prod_{m=1}^{p} (x - \bar{\lambda}_m).
\]

This \(\bar{q}\) is a real polynomial of degree \(p\), its leading coefficient is either 1 or \(-1\), and it satisfies conditions (13a) and (13b), furthermore its roots satisfy conditions (17a) and (18). The proof of this claim is analogous to the proof of Lemma 3.4

For convenience, we introduce the following notation. Let us denote the optimal SSP coefficient for explicit LM methods with \(k\) steps and order of accuracy \(p\) by \(C_{\text{exp}}(k, p)\), i.e.

\[
C_{\text{exp}}(k, p) = \sup_{k\text{-step explicit methods of order } p} C.
\]

Let us denote the optimal SSP coefficient for implicit LM methods with \(k\) steps and order of accuracy \(p\) by \(C_{\text{imp}}(k, p)\), i.e.

\[
C_{\text{imp}}(k, p) = \sup_{k\text{-step implicit methods of order } p} C.
\]

Lemmas 3.6–3.9 are the main results in this section.

**Lemma 3.6.** Let \(r \geq 0\) and let \(p, k\) be positive integers. Then the following statements are equivalent.

...
(i) $C_{\exp}(k, p) \leq r$.

(ii) There exists a non-zero polynomial $q$ of degree at most $p$, that satisfies conditions (13a)-(13b) and

$$q(0) = 0.$$  \hspace{1cm} (19)

Furthermore, if statement (i) holds, then the polynomial $q$ can be chosen to satisfy the following properties.

1. The degree of $q$ is exactly $p$.

2. The real parts of all roots of $q$ except for 0 lie in the interval $[1, k]$.

3. All real roots of $q$ are integers.

4. For even $p$, $k$ is a root of $q$ with odd multiplicity. For odd $p$, if $k$ is a root of $q$, then its multiplicity is even.

5. The multiplicity of the root 0 is one. For $1 \leq j \leq k - 1$, if $j$ is a root of $q$, then its multiplicity is 2.

Proof. First we show that statement (ii) implies statement (i). Suppose to the contrary that for some $p, k$ positive integers and $r = \rho_0 \geq 0$ the conditions of statement (ii) are fulfilled with $r = \rho$ by a polynomial $q(x) := c \cdot \prod_{m=1}^{p_0} (x - \lambda_m)$ of degree $0 < p_0 \leq p$, but there is nevertheless an explicit LMM of order $p$ with $k$ steps and with $C = \rho_1 > \rho_0$. We can assume without the loss of generality that $\lambda_1, \ldots, \lambda_{p_1} \neq 0$ and $\lambda_{p_1+1}, \ldots, \lambda_{p_0} = 0$, for some integer $0 \leq p_1 < p_0$. Let $0 < \epsilon < 1$ be sufficiently small so that $\frac{\epsilon}{1 - \epsilon} \leq \rho_1 - \rho_0$, and let us set

$$\tilde{q}(x) := \begin{cases} c \cdot \prod_{m=1}^{p_1} (x - \lambda_m) & \text{if } c \cdot \prod_{m=1}^{p_1} (-\lambda_m) < 0 \\ c \cdot (x - \epsilon) \prod_{m=1}^{p_1} (x - \lambda_m) & \text{if } c \cdot \prod_{m=1}^{p_1} (-\lambda_m) > 0 \end{cases}.$$  

This $\tilde{q}$ trivially satisfies conditions (13a) and (13c). The conditions of statement (ii) of Lemma 3.3 are also fulfilled by $\tilde{q}$ with $r = \rho_1$, since the same conditions are met by $q$ with $r = \rho_0$, and using the notations of Lemma 3.3 we have $\tilde{n}(j) = n(j)$ and

$$\rho_0 \geq \sum_{m=1}^{p_0} \frac{1}{j - \lambda_m} = \sum_{m=1}^{p_1} \frac{1}{j - \lambda_m} + (p_0 - p_1) \frac{1}{j} \geq \sum_{m=1}^{p_1} \frac{1}{j - \lambda_m} + \frac{1}{j - \epsilon} - \frac{\epsilon}{j(j - \epsilon)}$$

for all $1 \leq j \leq k$. Hence, in view of Lemma 3.3 $\tilde{q}$ satisfies conditions (13a)-(13c) with $r = \rho_1$, therefore Lemma 3.1 implies that $C < \rho_1$. This contradicts our initial assumption, so we can conclude that statement (ii) implies statement (i).

Now we show that statement (i) implies statement (ii). Let $k, p$ be arbitrary positive integers. In view of Lemma 3.1 and Lemma 3.4 there exists a real sequence $(r_n)$ with $\lim_{n \to \infty} r_n =$
Lemma 3.7. Let \( r \geq 0 \) and let \( p, k \) be positive integers. Then the following statements are equivalent.

---

\[ (q_n(x)) := (c \cdot \prod_{m=1}^{p} (x - \lambda_{m,n})) \]

such that for all \( n \) positive integers, \( q_n \) satisfies all the conditions listed in Lemma 3.4 with \( r = r_n \). Since \( (\lambda_{1,n}, \ldots, \lambda_{p,n}) \in \mathcal{H}^p \) for all \( n \) and since the set \( \mathcal{H}^p \subset \mathbb{C}^p \) is closed and bounded, the Bolzano–Weierstrass theorem guarantees that for an appropriate increasing sequence of indices \( n_1 < n_2 < \ldots \) the limit \( \lambda_m := \lim_{j \to \infty} \lambda_{m,n_j} \) exists and \( \lambda_m \in \mathcal{H} \) for all \( 1 \leq m \leq p \). A simple continuity argument shows that the polynomial \( q(x) := c \cdot \prod_{m=1}^{p} (x - \lambda_m) \) satisfies all the conditions set out in statement (ii).

In a few steps we transform this \( q \) into a polynomial \( \tilde{q} \) that fulfills the same conditions, and also satisfies Properties 1–5 of the Lemma.

**Step 1.** First we set

\[
\bar{\lambda}_{m,0} := \begin{cases} 
\left\lfloor \frac{\lambda_m}{m} \right\rfloor & \text{if } 1 \leq m \leq p \text{ and } \lambda_m \in \mathbb{R} \\
\lambda_m & \text{if } 1 \leq m \leq p \text{ and } \lambda_m \notin \mathbb{R}
\end{cases}

\tilde{q}_0(x) := c \cdot \prod_{m=1}^{p} (x - \bar{\lambda}_{m,0}).
\]

Replacing some non-integer real roots with their integer parts does not decrease the multiplicity of any positive integer roots, it does not change the value of \( n(j) \) and it does not increase the value of the left-hand-side of (16b) for any \( 1 \leq j \leq k \), therefore in view of statements (i) and (ii) of Lemma 3.3, \( \tilde{q}_0 \) satisfies conditions (13a) and (13b), and \( \tilde{q}_0 \) clearly satisfies condition (19).

**Step 2.** Next we take indices \( 1 \leq j \leq k \) in descending order. For each \( j \) if \( j \) is a root of \( \tilde{q}_{k-j} \) with multiplicity \( s > 2 \) then we set the multiplicity of \( j \) to be 2 by replacing \( s - 2 \) of these roots with \( j - 1 \); we denote the resulting polynomial by \( \tilde{q}_{k-j+1} \). A similar argument shows that \( \tilde{q}_{k+1} \) satisfies conditions (13a)–(13b) and (19).

**Step 3.** Now if \( 0 \) is a root of \( \tilde{q}_k \) with multiplicity \( s > 1 \), then we keep \( 0 \) as a single root, increase the multiplicity of \( k \) by \( s - 1 \), and multiply \( c \) by \((-1)^{s-1}\). For all \( \lambda \) roots with \( 0 < \text{Re}(\lambda) < 1 \) we replace \( \lambda \) with \( k \), and denote the resulting polynomial by \( \tilde{q}_{k+1} \). Again a simple argument shows that \( \tilde{q}_{k+1} \) satisfies conditions (13a)–(13b) and (19).

**Step 4.** If \( \tilde{q}_{k+1} \) has no simple real roots, then we set \( \tilde{q} := \tilde{q}_{k+1} \).

Otherwise \( j_0 \) is a single root of \( \tilde{q}_{k+1} \) for some \( 1 \leq j_0 \leq k - 1 \). We show that for all \( j_0 < j \leq k \) indices \( j \) is a multiple root of \( \tilde{q}_{k+1} \). This holds, because if it was not the case, then let \( j_1 \) denote the smallest integer \( j_0 \leq j < k \) such that either \( j \) is a single root of \( \tilde{q}_{k+1} \) or \( j \) is not a root of \( \tilde{q}_{k+1} \). Clearly \( n(j_0) = -n(j_1) \) since all real roots of \( \tilde{q}_{k+1} \) are integers, and \( j \) is a double root of \( \tilde{q}_{k+1} \) for all \( j_0 < j < j_1 \). Therefore in view of Lemma 3.3, conditions (13a) and (13b) cannot hold for both \( j = j_0 \) and \( j = j_1 \). Now we decrease the multiplicity of the \( k \) by one and increase the multiplicity of \( j_0 \) by one, and denote the resulting polynomial by \( \tilde{q} \). Using Lemma 3.3 one can easily show that \( \tilde{q} \) fulfills conditions (13a)–(13b) and (19).

By construction, Properties 1–3 and 5 trivially hold for \( \tilde{q} \), and Property 4 is just a simple consequence of said properties and the Conjugate root theorem. \( \square \)

**Lemma 3.7.** Let \( r \geq 0 \) and let \( p, k \) be positive integers. Then the following statements are equivalent.
\( C_{\text{imp}}(k, p) \leq r. \)

(ii) There exists a non-zero polynomial \( q \) of degree at most \( p \), that satisfies conditions (13a) – (13b) and (19) and

\[ q'(0) = 0. \]  

(20)

Furthermore, if statement (i) holds, then the polynomial \( q \) can be chosen to satisfy the following properties.

1. The degree of \( q \) is exactly \( p \).
2. The real parts of all roots of \( q \) except for 0 lie in the interval \([1, k]\).
3. All real roots of \( q \) are integers.
4. For odd \( p \), \( k \) is a root of \( q \) with odd multiplicity. For even \( p \), if \( k \) is a root of \( q \), then its multiplicity is even.
5. The multiplicity of the root 0 is two. For \( 1 \leq j \leq k - 1 \), if \( j \) is a root of \( q \), then its multiplicity is 2.

Proof. The proof of this lemma is similar to the proof of Lemma 3.6.

Lemma 3.8. Let positive integers \( k, p \) be such that \( 0 < C_{\text{exp}}(k, p) < \infty \). Suppose that \((\delta_j)_{j=0}^{k-1}\) and \((\beta_j)_{j=0}^{k-1}\) are the coefficients of an explicit LM method of order \( p \) with \( k \) steps and with SSP coefficient \( C = C_{\text{exp}}(k, p) \); suppose further that \( q \) is a polynomial that satisfies conditions (13a), (13b) and (19) with \( r = C_{\text{exp}}(k, p) \). Then the following statements hold.

(i) If \( \delta_j \neq 0 \) for some \( 0 \leq j \leq k - 1 \), then \( q(k - j) = 0. \)

(ii) If \( \beta_j \neq 0 \) for some \( 0 \leq j \leq k - 1 \), then \( q'(k - j) + C_{\text{exp}}(k, p)q(k - j) = 0 \).

(iii) This \( q \) can be chosen so that the total number of binding inequalities in (13a)–(13b) is at least \( p \), moreover \( q \) satisfies Properties 1–5 of Lemma 3.6.

Proof. Suppose that integers \( k, p > 0 \), coefficients \((\delta_j)_{j=0}^{k-1}\), \((\beta_j)_{j=0}^{k-1}\) and the polynomial \( q \) satisfy the conditions of the lemma. Let us consider the following primal–dual pair of LP problems.

Maximize 0 subject to \((\delta_j)_{j=0}^{k-1}, (\beta_j)_{j=0}^{k-1}\) satisfy (2) with \( r = C_{\text{exp}}(k, p) \). (21)

Minimize \( \sum_{m=0}^{p} k^m y_m \) subject to (12a) and (12b) with \( r = C_{\text{exp}}(k, p) \). (22)

Due to the assumptions made in the lemma, \((\delta_j)_{j=0}^{k-1}, (\beta_j)_{j=0}^{k-1}\) is a feasible solution to (21), and \( y = 0 \) is a feasible solution to (22). Hence both (21) and (22) are feasible, and thus the Duality theorem in LP (Proposition 3.2) implies that the two optima are equal, i.e. a feasible solution to (22) is optimal if and only if \( \sum_{m=0}^{p} k^m y_m = 0. \)
Let us set $y_m := (-1)^m q^{(m)}(k)$ for $0 \leq m \leq p$. Then $(y_m)^p_{m=0}$ satisfy condition (12a), since $q$ satisfies condition (13a) and $\sum_{m=0}^p y_m = \sum_{m=0}^p ((k-j) - k)^m q^{(m)}(k) = q(k-j) \geq 0$ for all $0 \leq j \leq k-1$. Similarly $(y_m)^p_{m=0}$ satisfy condition (12b) with $r = \exp(k,p)$, since $q$ satisfies condition (13b) with $r = \exp(k,p)$ and $\sum_{m=0}^p (m^{j=0} y_m + \exp(k,p) y_m) = \sum_{m=0}^p (-m((k-j) - k)^{m-1} + \exp(k,p)((k-j) - k)^m q^{(m)}(k) = -q(k-j) + \exp(k,p) q(k-j) \geq 0$ for all $0 \leq j \leq k-1$. It is also true that $\sum_{m=0}^p k^m y_m = 0$ as a consequence of $q(0) = 0$, therefore this $(y_m)^p_{m=0}$ is an optimal solution to the LP problem (22).

Now suppose that $\delta_j \neq 0$ for some $1 \leq j \leq k$. Then the Complementary slackness theorem (Proposition 3.3) implies that $0 = \sum_{m=0}^p m^j y_m = q(k-j)$. Similarly, in view of the Complementary slackness theorem, $\beta_j \neq 0$ implies $q(k-j) + \exp(k,p) q(k-j) = 0$. Hence the proofs of statements (i) and (ii) are complete.

Now we prove statement (iii). Suppose that the conditions of the lemma hold, suppose further that a non-zero $q$ is chosen so that the number of binding inequalities in (13a–13b) is maximal. Let $(y_m)^p_{m=0}$ be defined as before, and let the set of indices corresponding to the binding inequalities in (12a) and in (12b) be denoted by $I$ and $J$, respectively.

There is at least one inequality in (12a–12b) that does not hold with equality. Indeed, suppose to the contrary that $I = \{1,2,\ldots,k\}$ and $J = \{1,2,\ldots,k\}$. Then one can easily check that $j$ is a multiple root of $q$ for all $1 \leq j \leq k$; therefore the lemma contradicts the assumptions of the lemma.

The rank of the matrix of the system formed by the linear equations corresponding to the binding inequalities in (12a–12b) and by the equation $\sum_{m=0}^p y_m k^m = 0$ is exactly $p$. The rank of the matrix is clearly at most $p$, as the system is homogeneous and consistent. Suppose to the contrary that the rank the matrix is less then $p$. Since not all inequalities in (12a–12b) are binding, by continuity one can find a $(\tilde{y}_m)^p_{m=0}$ solution to the LP problem (22), such that $(\tilde{y}_m)^p_{m=0}$ and $(y_m)^p_{m=0}$ are linearly independent and the inequalities corresponding to indices in $I$ and $J$ hold with equality for $(\tilde{y}_m)^p_{m=0}$. One can easily check that $\tilde{q} := \sum_{m=0}^p \tilde{y}_m (k-x)^m$ is not a multiple of $q$, but it satisfies conditions (13a–13b) and (19), moreover if $q$ satisfies an inequality in (13a–13b) with equality, then the same equality is also satisfied by $\tilde{q}$. Hence by continuity, for appropriate $a_0, a_1 \in \mathbb{R}$ coefficients, the polynomial $q_0 := a_0 q + a_1 \tilde{q}$ satisfies conditions (13a, 13b) and (19), and the number of binding inequalities in (13a–13b) is greater for $\tilde{q}$ than for $q$. This contradicts the assumptions made on $q$.

Now we show that the number of binding inequalities in (12a–12b) is at least $p$. Suppose that the opposite is true, and the number of binding inequalities is at most $p-1$. Due to the previous step, this number is exactly $p-1$. Then by continuity there is a non-zero $(y_m)^p_{m=0}$ solution to the system of linear equations formed by the binding inequalities in (12a–12b) and by $\sum_{m=0}^p y_m k^m = 0$ with $r = r_0$ for some $0 < r_0 < \exp(k,p)$, that satisfies the conditions (12a) and (12b) with $r = r_0$ for all $0 \leq j \leq k-1$. One can check that the non-zero polynomial $\tilde{q} := \sum_{m=0}^p \tilde{y}_m (k-x)^m$ satisfies all the conditions of Lemma 3.6 with $r = r_0$, therefore the lemma implies the contradiction $\exp(k,p) \leq r_0$.
As a result of the above, \( q \) satisfies at least \( p \) inequalities in (13a)–(13b) with equality. Now let us apply the transformations found in the proofs of Lemma 3.4 and Lemma 3.6 to \( q \), in order to get a polynomial \( \tilde{q} \) that satisfies all the conditions and properties listed in Lemma 3.6 with \( r = C_{\exp}(k, p) \). One can easily check that if any of the transformation steps changes the roots of \( q \), then the resulting polynomial satisfies the same conditions with \( r = r_0 \) for some \( 0 < r_0 < C_{\exp}(k, p) \), which again leads to a contradiction. Hence \( \tilde{q} := c \cdot q \) for some \( c > 0 \), therefore \( q \) also satisfies all the conditions and properties listed in Lemma 3.6 with \( r = C_{\exp}(k, p) \). This completes the proof of statement (iii).

Lemma 3.9. Let positive integers \( k, p \) be such that \( 0 < C_{\imp}(k, p) < \infty \). Suppose that \( (\delta_j)^{k-1}_{j=0} \) and \( (\beta_j)^{k-1}_{j=0} \) are the coefficients of an implicit LM method of order \( p \) with \( k \) steps and with SSP coefficient \( C = C_{\imp}(k, p) \), suppose further that \( q \) is a polynomial that satisfies conditions (13a)–(13b), (19) and (20) with \( r = C_{\imp}(k, p) \). Then the following statements hold.

(i) If \( \delta_j \neq 0 \) for some \( 0 \leq j \leq k - 1 \), then \( q(k - j) = 0 \).

(ii) If \( \beta_j \neq 0 \) for some \( 0 \leq j \leq k - 1 \), then \( q'(k - j) + C_{\imp}(k, p)q(k - j) = 0 \).

(iii) This \( q \) can be chosen so that the total number of binding inequalities in (13a)–(13b) is at least \( p - 1 \), moreover \( q \) satisfies Properties 1–5 of Lemma 3.7.

Proof. The proof follows the same argumentation as the proof of Lemma 3.8

4 Upper bounds on SSP coefficients

In this section we derive upper bounds on SSP coefficients using Lemma 3.6 and Lemma 3.7. Proposition 4.1 is just the classical upper bound on the SSP coefficient for explicit LM methods, found in [Len89].

Proposition 4.1. Let \( k, p \) be positive integers. Then the following inequality holds.

\[
C_{\exp}(k, p) \leq \begin{cases} 
\frac{k-p}{k-1} & \text{if } k \geq 2 \text{ and } k \geq p \\
0 & \text{if } k < p \\
1 & \text{if } k = p = 1.
\end{cases}
\]

Proof. Let us consider \( q(x) := x(k - x)^{p-1} \), a polynomial of degree \( p \). If \( k \geq 2 \) then \( q \) satisfies the conditions (13a)–(13b) and (19) with \( r = \max \left( \frac{k-p}{k-1}, 0 \right) \). If \( k = 1 \) and \( p \geq 2 \) then \( q \) satisfies the same conditions with \( r = 0 \). Finally, if \( p = k = 1 \) then \( q \) satisfies the same conditions with \( r = 1 \). The statement of the proposition is an immediate consequence of Lemma 3.6.

Theorem 4.1 can be viewed as an extension of the upper bound \( C_{\imp}(k, p) \leq 2 \) for all \( k \geq 1 \) and \( p \geq 2 \) proved in [Len91][HR05].
Theorem 4.1. Let \( k \geq 1 \) and \( p \geq 2 \) be arbitrary integers. Then the following inequality holds.

\[
C_{\text{imp}}(k, p) \leq \begin{cases} 
\frac{2k-p}{k-1} & \text{if } k \geq 2 \text{ and } 2k \geq p \\
0 & \text{if } 2k < p \\
2 & \text{if } k = 1 \text{ and } p = 2.
\end{cases}
\]

Proof. Let us consider \( q(x) := x^2(k - x)^{p-2} \), a polynomial of degree \( p \). If \( k \geq 2 \) then \( q \) satisfies conditions (13a)(13b), (19) and (20) with \( r = \max \left( \frac{2k-p}{k-1}, 0 \right) \). If \( k = 1 \) and \( p \geq 3 \) then \( q \) satisfies the same conditions with \( r = 0 \). Finally, if \( k = 1 \) and \( p = 2 \) then \( q \) satisfies the same conditions with \( r = 2 \). The statement of the theorem is an immediate consequence of Lemma 3.7.

Proposition 4.2. The following statements hold.

(i) Suppose that \( p, k \geq 1 \) and \( C_{\text{exp}}(k, p) > 0 \). Then there exists an explicit LM method of order \( p \) with \( k \) steps, and with \( C = C_{\text{exp}}(k, p) \).

(ii) Suppose that \( p \geq 2 \), \( k \geq 1 \) and \( C_{\text{imp}}(k, p) > 0 \). Then there exists an implicit LM method of order \( p \) with \( k \) steps, and with \( C = C_{\text{imp}}(k, p) \).

Proof. The proof of statement (i) is based on Lemma 3.1 and Proposition 4.1, and on the fact that if a polynomial \( q \) solves the system (13) with \( r = r_0 > 0 \), then the polynomial \( \tilde{q} := q + |q(0)|/2 \) solves the same system with \( r = r_1 \) for some \( 0 < r_0 < r_1 \). Similarly, the proof of statement (ii) is based on Lemma 3.2 and Theorem 4.1.

Theorem 4.2 presents a relation between the optimal SSP coefficients for explicit and implicit LM methods of different orders. This inequality, together with the existence of arbitrary order implicit LM methods with \( C > 0 \) proved in [San86], implies the existence of arbitrary order LM methods with \( C > 0 \). However, Theorem 5.1 proves the existence of explicit LM methods with \( C > 0 \) for a much lower number of steps.

Theorem 4.2. Let \( k, p \) be positive integers. Then the following inequality holds.

\[
C_{\text{imp}}(k, 2p) \leq 2C_{\text{exp}}(k, p)
\]

Proof. In view of Lemma 3.6, there exists a polynomial of degree \( p \) that satisfies conditions (13a)–(13b) and (19) with \( r = C_{\text{exp}}(k, p) \). Let us denote this polynomial by \( q \). Then the polynomial \( \tilde{q} := q^2 \) is a real polynomial of degree \( \tilde{p} := 2p \). One can easily show that \( \tilde{q} \) satisfies conditions (13a), (19) and (20).

This \( \tilde{q} \) also satisfies condition (13b) with \( r = 2C_{\text{exp}}(k, p) \), since 

\[
-\tilde{q}'(j) + 2C_{\text{exp}}(k, p)\tilde{q}(j) = 2q(j) \left( -q'(j) + C_{\text{exp}}(k, p)q(j) \right) \geq 0
\]

for all \( 1 \leq j \leq k \) because of the aforementioned properties of \( q \). Thus \( \tilde{q} \) satisfies all the conditions of statement (ii) of Lemma 3.7, therefore statement (i) of the Lemma holds, and that gives (23).
5 Existence of arbitrary order SSP explicit LMMs

In [Len89, Theorem 2.3(ii)], it is asserted that there exist explicit contractive linear multistep methods of arbitrarily high order; the justification cited is [San86, Theorem 2.3]. The latter Theorem does prove existence of arbitrary-order contractive linear multistep methods; however, it uses an assumption that if \( \alpha_j \neq 0 \) for some \( j \), then also \( \beta_j \neq 0 \), which cannot hold for explicit methods (since necessarily \( \alpha_k \neq 0 \) and \( \beta_k = 0 \)). Hence the methods constructed there are necessarily implicit.

In view of Lemma 3.6, the existence of arbitrary-order SSP explicit LMMs can be shown by proving the infeasibility of (13a), (13b) and (19) with \( r = 0 \) and a large enough \( k \) for all \( p \). This can be achieved by applying Markov brothers-type inequalities to the polynomial \( q \). These inequalities give bounds on the maximum of the derivatives of a polynomial over an interval in terms of the maximum of the polynomial, and they are widely applied in approximation theory.

**Proposition 5.1** (Markov brothers’ inequality [Mar90, Mar92]). Let \( P \) be a real univariate polynomial of degree \( n \). Then

\[
\max_{-1 \leq x \leq 1} |P^{(\ell)}(x)| \leq \frac{n^2(n^2 - 1^2)(n^2 - 2^2) \cdots (n^2 - (\ell - 1)^2)}{1 \cdot 3 \cdot 5 \cdots (2\ell - 1)} \max_{-1 \leq x \leq 1} |P(x)|
\]

for all \( \ell \) positive integers.

**Theorem 5.1.** Let \( p > 0 \) and

\[
k > \sqrt{\frac{p^2(p^2 - 1)}{6} \cdot \left\lfloor \frac{p + 2}{2} \right\rfloor}.
\]

be arbitrary integers. Then \( C_{\exp}(k, p) > 0 \), i.e. there exist explicit LM methods with \( k \) steps, order of accuracy \( p \) and \( C > 0 \).

**Proof.** Assume to the contrary that \( C_{\exp}(k, p) = 0 \) for some \( p \) and \( k \) satisfying (24). Then Lemma 3.6 implies the existence of a real polynomial \( q \) of degree \( p \) that satisfies conditions (13a), (13b) and (19) with \( r = 0 \), furthermore properties 1–5 of Lemma 3.6 are fulfilled by \( q \). Due to (3.6) and properties 3, 5 of the Lemma, \( q(x) \geq 0 \) for all \( x \in [0, k] \). Let us use the following notation:

\[
a = \max_{x \in [0,k]} |q(x)| \quad \quad b = \max_{x \in [0,k]} |q''(x)|.
\]

First we introduce the polynomial \( P(x) := q((x + 1)^2) - \frac{q}{2} \). Clearly \( \max_{x \in [-1,1]} |P(x)| = \frac{1}{2}a \) due to \( \min_{x \in [0,k]} q(x) = 0 \) and \( \max_{x \in [-1,1]} |P''(x)| = \frac{k^2}{4}b \). Applying the Markov brothers’ inequality (Proposition 5.1) with \( \ell = 2 \) to the polynomial \( P \) leads to

\[
b \leq a \cdot \frac{2p^2(p^2 - 1)}{3k^2}.
\]
Now since $q$ is a polynomial of degree $p - 1$ and $q'(j) \leq 0$ for all $1 \leq j \leq k$ due to (13b), hence

$$\left| \left\{ j : 0 \leq j \leq k - 1, \max_{x \in [j, j+1]} q'(x) > 0 \right\} \right| \leq \left\lceil \frac{p}{2} \right\rceil,$$

i.e. in the interval $[0, k]$, $q'$ takes positive values only within at most $\left\lceil \frac{p}{2} \right\rceil$ unit intervals defined by adjacent integers. Moreover, $q'(x) \leq b(1 - x)$ in the interval $[0, 1]$, and $q'(x) \leq b \cdot \max(|x|, |1 - x|)$ in the interval $[j, j+1]$ for $1 \leq j \leq k - 1$. Using these and (19), we obtain an upper estimate of $a$:

$$a \leq \int_0^k \max(q'(x), 0) \, dx \leq \frac{b}{2} + \frac{b}{4} \cdot \left\lceil \frac{p - 2}{2} \right\rceil = \frac{b}{4} \left\lceil \frac{p + 2}{2} \right\rceil.$$

(26)

Together (26) and (25) and $a > 0$ imply that

$$k \leq \sqrt{\frac{p^2(p^2 - 1)}{6} \cdot \left\lceil \frac{p + 2}{2} \right\rceil},$$

which contradicts our choice of $k$. This completes the proof.

\[\square\]

6 Asymptotic behavior of the optimal step size coefficient for large number of steps

Since for all positive $p$, $C_{\text{exp}}(k, p)$ and $C_{\text{imp}}(k, p)$ are trivially non-decreasing in $k$, the following definitions are meaningful.

$$C_{\text{exp}}(\infty, p) := \lim_{k \to \infty} C_{\text{exp}}(k, p) \quad \quad C_{\text{imp}}(\infty, p) := \lim_{k \to \infty} C_{\text{imp}}(k, p)$$

Due to the existence of arbitrary order explicit and implicit LM methods with $C > 0$, and due to the upper bounds on SSP coefficients described in Proposition 4.1 and Theorem 4.1, $C_{\text{exp}}(\infty, p) \in (0, 1]$ for all positive $p$ and $C_{\text{imp}}(\infty, p) \in (0, 2]$ for all $p \geq 2$.

**Theorem 6.1.** Let $p$ be a positive integer. Then the following statements hold.

(i) If $p$ is odd then there exists a positive integer $K_p$ such that for all integers $k \geq K_p$

$$C_{\text{exp}}(k, p) = C_{\text{exp}}(\infty, p).$$

(ii) If $p$ is even then there exists a positive integer $k_p$ such that for all integers $k > k_p$

$$\frac{1}{k - 1} \leq C_{\text{exp}}(\infty, p - 1) - C_{\text{exp}}(k, p) \leq \frac{1}{k - k_p}.$$

(28)
Proof. For all positive integers \( p \) and \( n \leq p \), let \( L(p,n) \) denote the smallest whole number \( L \) such that for all \( k \geq 1 \) there exists a polynomial \( q(x) := c \cdot \prod_{m=0}^{p} (x - \lambda_m) \) that satisfies conditions (13a)–(13b) and (19) with \( r = C_{\exp}(k, p) \), fulfills all the properties listed in Lemma 3.6. Furthermore, its roots satisfy
\[
|\{m : 1 \leq m \leq p, \Re(\lambda_n) \in [0, L]\}| \geq n;
\] (29)
if no such \( L \) exist, then we define \( L(p,n) := \infty \). Let \( N(p) \) denote the largest \( n \leq p \) positive integer such that \( L(n,p) < \infty \). In view of the Conjugate root theorem, and due to properties 2,3 and 5 of Lemma (3.6), \( N(p) \) is odd for all positive \( p \).

**Step 1.** Let integers \( k \geq 2 \) and \( p \geq 1 \) be such that \( C_{\exp}(k,p) > 0 \), and let \( q \) be a polynomial that satisfies conditions (13a)–(13b) and (19) with \( r = C_{\exp}(k,p) \). One easily checks that the same conditions are satisfied with \( r = \max (0, r_0 - \frac{1}{k-1}) \) by the polynomial \( \tilde{q}(x) := (k-x) \cdot q(x) \), therefore in view of Lemma (3.6), \( C_{\exp}(k,p+1) \leq \max (0, C_{\exp}(k,p) - \frac{1}{k-1}) \). Hence \( C_{\exp}(k,p) \) is strictly decreasing in \( p \) until it reaches 0.

**Step 2.** Suppose that \( N(p) = p \) for some positive integer \( p \). Let us choose the positive integer \( K_p \) so that \( C_{\exp}(K_p,p) > 0 \), moreover \( K_p \geq L(p,p) + p/C_{\exp}(K_p,p) \). Such a \( K_p \) exists, because \( C_{\exp}(k,p) \) is non-decreasing in \( k \). Let \( q \) be a polynomial of degree \( p \) that satisfies conditions (13a)–(13b) and (19) with \( r = C_{\exp}(K_p,p) \) and \( k = K_p \), and whose roots fulfill condition (29) with \( L = L(p,p) \) and \( n = p \). This \( \tilde{q} \) clearly satisfies conditions (19) and (13a) for all \( j > K_p \). The inequality (13c) also holds with the same value of \( r \) for all \( j > K_p \), due to statement (ii) of Lemma (3.6), and
\[
\sum_{m=1}^{p} \frac{1}{j - \lambda_m} \leq \sum_{m=1}^{p} \frac{1}{j - \Re(\lambda_m)} < p \cdot \frac{1}{j - L(p,p)} \leq C_{\exp}(K_p,p).
\]
As a consequence of Lemma (3.6), \( C_{\exp}(k,p) \leq C_{\exp}(K_p,p) \) for all \( k \geq K_p \). Since \( C_{\exp}(k,p) \) is non-decreasing, \( C_{\exp}(k,p) = C_{\exp}(K_p,p) \) for all \( k \geq K_p \). Therefore \( C_{\exp}(\infty,p) = C_{\exp}(K_p,p) \) and condition (27) is satisfied. Hence for all positive \( p \), \( N(p) = p \) implies that condition (27) holds for an appropriate \( K_p \).

**Step 3.** Suppose that the assumptions of Step 2 hold for \( p \) and \( q \). Let us introduce the notation \( \mu := 1/C_{\exp}(\infty,p) \). Then the polynomial \( \tilde{q}(x) := (x^2 - 2(4\mu + L(p,p)) \cdot x + (4\mu + L(p,p))^2 + 4\mu^2) \cdot q(x) \) clearly satisfies conditions (19) and (13a) for all positive \( j \). Using the inequality \( \frac{1}{j-\lambda} + \frac{1}{\lambda} \leq \frac{1}{\Im(\lambda)} \), one can show in a similar way as in Step 2 that \( \tilde{q} \) satisfies condition (13b) with \( r = \frac{3}{4} C_{\exp}(\infty,p) \) for all \( j \geq L(p,p) + 2\mu \). Using that \( \frac{1}{j-\lambda} + \frac{1}{\lambda} \) is decreasing in \( j \) within the interval \( 1 \leq j \leq \Re(\lambda) - \Im(\lambda) \), one can easily show that condition (13b) is satisfied by \( \tilde{q} \) with \( r = C_{\exp}(\infty,p) - (L(p,p) + 4\mu)/((L(p,p) + 4\mu)^2 + 4\mu^2) \) for all \( 1 \leq j < L(p,p) + 2\mu \). Therefore, in view of Lemma (3.6), \( C_{\exp}(k,p+2) \) is bounded from above by the maximum of the above expressions for \( r \), e.g.
\[
C_{\exp}(\infty,p+2) \leq \max \left( \frac{3}{4} C_{\exp}(\infty,p), C_{\exp}(\infty,p) - \frac{L(p,p) + 4\mu}{(L(p,p) + 4\mu)^2 + 4\mu^2} \right).
\]
Hence for all positive \( p, N(p) = p \) implies that \( C_{\exp}(\infty, p) > C_{\exp}(\infty, p + 2) \).

**Step 4.** Suppose that \( N(p) = N(p_0) = p_0 \) for some \( p > p_0 \) positive integers, and let \( \epsilon > 0 \) be arbitrary. In view of Step 2, there exists a positive integer \( K_{p_0} \) such that \( C_{\exp}(k, p_0) = C_{\exp}(\infty, p_0) \) for all \( k \geq K_{p_0} \). Let us set \( L := \max(L(p, p_0), K_{p_0}) \) and \( K := L + (p - p_0)/\epsilon \). Since \( N(p) = p_0 \), there is an appropriate \( k > K \), so that there exists a \( q(x) := c \cdot \prod_{m=1}^{p_0} (x - \lambda_m) \) polynomial that satisfies conditions (13a–13b) and (19) with \( r = C_{\exp}(k, p) \), and that satisfies all the properties listed in Lemma 3.6, and whose roots satisfy the conditions \( \text{Re}(\lambda_1), \ldots, \text{Re}(\lambda_{p_0}) \in [0, L] \) and \( \text{Re}(\lambda_{p_0+1}), \ldots, \text{Re}(\lambda_p) \geq K \). Let us introduce the polynomial \( \tilde{q} := c(-1)^{p_0} \cdot \prod_{m=1}^{p_0} (x - \lambda_m)^{-1} \). This \( \tilde{q} \) is a polynomial of degree \( p_0 \) that satisfies the conditions of statements (i) of Lemma 3.3 for all positive \( j \), and also satisfies the conditions of statement (ii) of Lemma 3.3 with \( r = C_{\exp}(k, p) + \epsilon \) for all \( 1 \leq j \leq L \), since

\[
\sum_{m=0}^{p_0} \frac{1}{j - \lambda_m} = \sum_{m=0}^{p_0} \frac{1}{j - \lambda_m} + \sum_{m=p_0+1}^{p_0} \frac{1}{j - \lambda_m} \geq \sum_{m=0}^{p_0} \frac{1}{j - \lambda_m} + \frac{1}{K - L} = \sum_{m=0}^{p_0} \frac{1}{j - \lambda_m} - \epsilon
\]

for all \( 1 \leq j \leq L \). As a consequence of Lemma 3.6 and Lemma 3.3 \( C_{\exp}(k, p) + \epsilon \geq C_{\exp}(L, p_0) = C_{\exp}(k_{p_0}, p_0) = C_{\exp}(\infty, p_0) \). Since \( \epsilon > 0 \) is arbitrary and \( C_{\exp}(\infty, p) \) is nondecreasing in \( p, N(p) = N(p_0) = p_0 \) implies that \( C_{\exp}(\infty, p_0) = C_{\exp}(\infty, p_0) \).

Furthermore if \( p = p_0 + 1 \) then \( p \) is even, so property 4 of Lemma 3.6 guarantees that \( \lambda_p = k \). By following a similar argument we get that \( N(p) = N(p - 1) = p - 1 \) implies \( C_{\exp}(\infty, p - 1) = C_{\exp}(k, p) \).

**The proof of statement (ii) of the Theorem.** Clearly, \( N(1) = 1 \) holds.

Assume now that \( N(2j + 1) = 2j + 1 \) holds for all \( 0 \leq j \leq m - 1 \) integers. Since \( 1 \leq N(p) \leq p \) and \( N(p) \) is odd, we have \( N(2m + 1) = N(2j + 1) \) for some \( 0 \leq j_0 \leq m \). If \( j_0 < m \), then Step 4 implies that \( C_{\exp}(2m + 1) = C_{\exp}(2j_0 + 1) \), which contradicts the results of Step 3. Therefore \( N(2m + 1) = 2m + 1 \).

By induction we have \( N(p) = p \) for all positive odd integer values of \( p \). Now statement (i) of the Theorem is implied by Step 2.

**The proof of statement (ii) of the Theorem.** Let \( p \) be an arbitrary positive even integer. Then \( N(p) = p_0 \) for some positive odd integer \( p_0 \), since \( 1 \leq N(p) \leq p \) and \( N(p) \) is odd. Due to the previous step we have \( N(p_0) = p_0 \), thus Step 4 implies that \( C_{\exp}(\infty, p) = C_{\exp}(\infty, p_0) \). If \( p_0 = p - 1 \), then Step 3 implies that \( C_{\exp}(\infty, p) = C_{\exp}(\infty, p_0) = C_{\exp}(\infty, p - 1) \), which contradicts the fact that \( C_{\exp}(\infty, p) \) is non-increasing in \( p \). Therefore \( p_0 = p - 1 \), and as a consequence of Step 4 we have \( C_{\exp}(\infty, p - 1) - C_{\exp}(k, p) \leq \frac{1}{k - 1} \) holds for all \( k \geq 2 \) as a direct consequence of Step 1.

**Theorem 6.2.** Let \( p \geq 2 \) an arbitrary integer. Then the following statements hold.

(i) If \( p \) is even then there exists a positive integer \( K_p \) such that for all integers \( k \geq K_p \)
\[
C_{\text{imp}}(k, p) = C_{\text{imp}}(\infty, p).
\]
(ii) If $p$ is odd then there exists a positive integer $k_p$ such that for all integers $k > k_p$

$$\frac{1}{k - 1} \leq C_{\text{imp}}(\infty, p - 1) - C_{\text{imp}}(k, p) \leq \frac{1}{k - k_p}. \quad (31)$$

**Proof.** The proof is essentially the same as the proof of Theorem 6.1. \qed

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