Positivity of exponential multistep methods

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Summary. In this paper, we consider exponential integrators that are based on linear multistep methods and study their positivity properties for abstract evolution equations. We prove that the order of a positive exponential multistep method is two at most and further show that there exist second-order methods preserving positivity.

1 Introduction

Integration schemes that involve the evaluation of the exponential were first proposed in the 1960s for the numerical approximation of stiff ordinary differential equations. Nowadays, due to advances in the computation of the product of a matrix exponential with a vector, such methods are considered as practicable also for high-dimensional systems of differential equations. The renewed interest in exponential integrators is further enhanced by recent investigations which showed that they have excellent stability and convergence properties. In particular, they perform well for differential equations that result from a spatial discretisation of nonlinear parabolic and hyperbolic initial-boundary value problems, see [4, 9] and references therein.

However, aside from a favourable convergence behaviour, the usability of a numerical method for practical applications is substantially affected by its qualitative behaviour, and, in many cases, it is inevitable to ensure that certain geometric properties of the underlying problem are well preserved by the discretisation. In particular, it is desirable that the positivity of the true solution is retained by the numerical approximation. More precisely, if the solution of a linear abstract evolution equation

$$u'(t) = A\,u(t) + f(t), \quad 0 < t \le T, \qquad u(0) \text{ given}, \tag{1}$$

remains positive, the numerical solution should retain this property. Unfortunately, as proven by Bolley and Crouzeix [3], the order of positive rational one-step and linear multistep methods, respectively, is restricted by one.

The objective of the present paper is to investigate exponential multistep methods where the coefficients are combinations of the exponential and closely related functions. The general form of the considered schemes is introduced below in Section 3. Examples include Adams-type methods that were studied recently in [4, 9] for parabolic problems, see also the earlier works [8, 12].

The main result, which we deduce in Section 4, states that positive exponential multistep methods are of order two at most. Further, we show that there exist second-order methods which preserve positivity. Thus, the order barrier of [3] is raised by one. For exponential Runge–Kutta methods, a similar result has been obtained recently in [10].

Our analysis of exponential multistep methods for abstract evolution equations is based on an operator calculus which allows to define the Laplace-Stieltjes transform involving the generator of a positive C_0-semigroup. We refer to the subsequent Section 2, where the basic hypotheses on the differential equation and some fundamental tools of the employed analytical framework are recapitulated.

2 Analytical framework

In this section, we state the basic assumptions on the abstract initial value problem (1).

Throughout, we let $\big(V, \|\cdot\|\big)$ denote the underlying Banach space. Further, we suppose $A : D \subset V \to V$ to be a densely defined and closed linear operator on V that generates a *strongly continuous* semigroup $\big(\mathrm{e}^{tA}\big)_{t\geq 0}$ of type (M,ω), that is, there exist constants $M \geq 1$ and $\omega \in \mathbb{R}$ such that the bound

$$\big\|\mathrm{e}^{tA}\big\| \leq M\mathrm{e}^{t\omega}, \qquad t \geq 0, \tag{2}$$

is valid. For a detailed treatment of C_0-semigroups, we refer to the monographs [6, 11].

The notion of positivity requires the Banach space V to be endowed with an additional order structure. In the present paper, to keep the analytical framework simple, we restrict ourselves to the consideration of the Lebesgue spaces and subspaces thereof, respectively, as it is then straightforward to define the positivity of an element pointwise.[1] In general, an appropriate setting is provided by the theory of Banach lattices treated in Yosida [13, Chap. XII]. Our results remain valid within this framework.

We recall that a bounded linear operator $B : V \to V$ is said to be *positive* if for any element $v \in V$ satisfying $v \geq 0$ it follows $Bv \geq 0$.

[1] A function $v : \Omega \subset \mathbb{R}^d \to \mathbb{R}$ in $\mathrm{L}^p(\Omega)$, $1 \leq p \leq \infty$, is said to be *positive* if it is pointwise positive, i.e., $v(x) \geq 0$ for almost all $x \in \Omega$. In that case, we write $v \geq 0$ for short. We employ here the standard terminology, although the term *non-negative* would be more appropriate.

Example 1. We consider the differential operator ∂_{xx} subject to a mixed boundary condition on the Banach space of continuous functions, that is, for some $c_1, c_2 \in \mathbb{R}$ we set $A : D \to V : v \mapsto \partial_{xx} v$ where $V = \mathrm{C}([0,1])$ and $D = \{v \in \mathrm{C}^2([0,1]) : v'(0) + c_1 v(0) = 0 = v'(1) + c_2 v(1)\}$. It is shown in Arendt et al. [1, p. 134] that the associated semigroup $\left(\mathrm{e}^{tA}\right)_{t\geq 0}$ is positive.

Henceforth, we assume that the linear operator $A : D \to V$ is the generator of a positive semigroup $\left(\mathrm{e}^{tA}\right)_{t\geq 0}$ of type (M, ω), see (2). Then, from the formulation of the linear evolution equation (1) as a Volterra integral equation

$$u(t) = \mathrm{e}^{tA}\, u(0) + \int_0^t \mathrm{e}^{(t-\tau)A} f(\tau)\, \mathrm{d}\tau, \qquad 0 \leq t \leq T, \tag{3}$$

it is seen that the solution u remains positive, provided that the initial value $u(0)$ and the function f are positive.

Let $a \in \mathrm{BV}$ denote a function of bounded variation that is normalised at its discontinuities and satisfies $a(0) = 0$. The associated *Laplace-Stieltjes transform* is defined through

$$G(z) = \int_0^\infty \mathrm{e}^{tz}\, \mathrm{d}a(t), \tag{4}$$

see Hille and Phillips [6, Sect. 6.2]. We recall that a real-valued function G is said to be *absolutely monotonic* on an interval $I \subset \mathbb{R}$ if

$$G^{(j)}(x) \geq 0, \qquad x \in I, \quad j \geq 0.$$

The following result by Bernstein [2], which characterises absolutely monotonic functions of the form (4), is the basis of our analysis in Section 4.

Theorem 1 (Bernstein). *A function G is absolutely monotonic on the half line $(-\infty, \omega]$ iff it is the Laplace-Stieltjes transform of a non-decreasing function $a \in \mathrm{BV}$ such that*

$$\int_0^\infty \mathrm{e}^{t\omega}\, |\mathrm{d}a(t)| < \infty.$$

A well-known operational calculus described in Hille and Phillips [6, Chap. XV] allows to extend (4) to unbounded linear operators. More precisely, for A being the generator of a strongly continuous semigroup $\left(\mathrm{e}^{tA}\right)_{t\geq 0}$ on V, it holds

$$G(hA)\, v = \int_0^\infty \mathrm{e}^{thA}\, v\, \mathrm{d}a(t), \qquad h \geq 0, \quad v \in V, \tag{5}$$

where the integral is defined in the sense of Bochner. It is thus straightforward to deduce the following corollary from Theorem 1, see also Kovács [7].

Corollary 1. *Suppose that the linear operator A generates a positive and strongly continuous semigroup of type (M, ω). Assume further that the function G is absolutely monotonic on $(-\infty, h\omega]$ for some $h \geq 0$. Then, the linear operator $G(hA)$ defined by (5) is positive.*

Remark 1. We note that the converse of the above corollary is true as well. Namely, if $G(hA)$ is positive for any generator A of a positive and strongly continuous semigroup, then the function G is absolutely monotonic. The proof of this statement is in the lines of Bolley and Crouzeix [3, Proof of Lemma 1].

The construction of exponential integrators often relies on the variation-of-constants formula (3) and a replacement of the integrand f by an interpolation polynomial. As a consequence, the linear operators $\varphi_j(hA)$ defined through

$$\varphi_j(z) = \int_0^1 \mathrm{e}^{tz} \, \frac{(1-t)^{j-1}}{(j-1)!} \, \mathrm{d}t, \qquad j \geq 1, \qquad z \in \mathbb{C}, \tag{6}$$

naturally arise in the numerical schemes. By the above Theorem 1, these functions are absolutely monotonic, and thus the positivity of the associated operators $\varphi_j(hA)$ follows from Corollary 1.

3 Exponential multistep methods

In this section, we introduce the considered exponential multistep methods for the time integration of the linear evolution equation (1) and state the order conditions. The positivity properties of the numerical schemes are then studied in Section 4.

We let $t_j = jh$ denote the grid points associated with a constant stepsize $h > 0$. Besides, we suppose that the starting values $u_0, u_1, \dots, u_{k-1} \in V$ are approximations the exact solution values of (1). Then, for integers $j \geq k$, the numerical solution values $u_j \approx u(t_j)$ are given by the k-step recursion

$$\sum_{\ell=0}^{k} \alpha_\ell(hA) \, u_{n+\ell} = h \sum_{\ell=0}^{k} \beta_\ell(hA) \, f(t_{n+\ell}), \qquad n \geq 0. \tag{7a}$$

Throughout, we choose $\alpha_k = 1$. Furthermore, we assume that the coefficient functions α_ℓ and β_ℓ are given as Laplace-Stieltjes transforms of certain functions a_ℓ and b_ℓ. Thus, it holds

$$\alpha_\ell(z) = \int_0^\infty \mathrm{e}^{tz} \, \mathrm{d}a_\ell(t), \quad \beta_\ell(z) = \int_0^\infty \mathrm{e}^{tz} \, \mathrm{d}b_\ell(t), \qquad z \in (-\infty, \omega]. \tag{7b}$$

For simplicity, we require b_ℓ to be piecewise differentiable such that the left-sided limit of $b_\ell'(t)$ exist at $t = j$ for all integers $j \geq 0$. In particular, these assumptions are satisfied if the coefficients functions are (linear) combinations of the exponential and the related φ-functions (6). We therefore refer to (7) as an *exponential linear k-step method*. Due to (7b), the operators $\alpha_\ell(hA)$ and $\beta_\ell(hA)$ are bounded on V.

Examples that have recently been studied in literature for the time integration of semilinear evolution equations are exponential Adams-type methods. For the choice $\alpha_1 = \ldots = \alpha_{k-1} = 0$ and $\beta_k = 0$, the resulting methods are discussed in Calvo and Palencia [4]. On the other hand, the case

$\alpha_0 = \ldots = \alpha_{k-2} = 0$ and $\beta_k = 0$ generalising the classical Adams–Bashforth methods is covered by the analysis given in [9].

In the following, we derive the order conditions for the exponential k-step method. We note that the arguments given below extend to semilinear problems $u'(t) = A\,u(t) + F\big(t, u(t)\big)$ by setting $f(t) = F\big(t, u(t)\big)$. As usual, the numerical method (7) is said to be *consistent* of order p, if the local error

$$d(t,h) = \sum_{\ell=0}^{k} \alpha_\ell(hA)\,u(t+\ell h) - h \sum_{i=0}^{k} \beta_\ell(hA)\,f(t+\ell h) \tag{8}$$

is of the form $d(t,h) = \mathscr{O}\big(h^{p+1}\big)$ for $h \to 0$, provided that the function f is sufficiently smooth, see Hairer, Nørsett, and Wanner [5, Chap. III.2].

In order to determine the leading h-term in $d(t,h)$, we make use of the variation-of-constants formula

$$u(t+\ell h) = \mathrm{e}^{\ell h A}\,u(t) + \int_0^{\ell h} \mathrm{e}^{(\ell h - \tau)A}\,f(t+\tau)\,\mathrm{d}\tau,$$

see also (3). We expand all occurrences of f in Taylor series at t and apply the definition of the φ-functions (6). A comparison in powers of h finally yields the following result.

Lemma 1. *The order conditions for exponential multistep methods* (7) *are*

$$\sum_{\ell=0}^{k} \alpha_\ell(hA)\,\mathrm{e}^{\ell h A} = 0, \tag{9a}$$

$$\sum_{\ell=1}^{k} \alpha_\ell(hA)\,\ell^q\,\varphi_q(\ell h A) \;=\; \sum_{\ell=0}^{k} \beta_\ell(hA)\,\frac{\ell^{q-1}}{(q-1)!}, \qquad 1 \le q \le p, \tag{9b}$$

where by definition $\ell^0 = 1$ *for* $\ell = 0$.

The first condition corresponds to the requirement that the exponential multistep method (7) is exact for the homogeneous equation $u'(t) = A\,u(t)$. By setting $A = 0$ in (9), the usual order conditions

$$\sum_{\ell=0}^{k} \alpha_\ell(0) = 0, \qquad \sum_{\ell=1}^{k} \alpha_\ell(0)\,\ell^q = q \sum_{\ell=0}^{k} \beta_\ell(0)\,\ell^{q-1}, \quad 1 \le q \le p$$

for a linear multistep method with coefficients $\alpha_\ell(0)$ and $\beta_\ell(0)$ follow, see also [5, Chap. III.2].

4 Positivity and order barrier

In this section, we derive an order barrier for positive exponential multistep methods. According to Bolley and Crouzeix [3], the numerical method (7) is said to be *positive*, if the numerical solution values u_n remain positive for all $n \geq k$, provided that the semigroup $\big(\mathrm{e}^{tA}\big)_{t\geq 0}$, the function f, and further the starting values $u_0, u_1, \dots, u_{k-1}$ are positive. We note that the requirement of positivity implies that the coefficients operators $\alpha_\ell(hA)$ satisfy

$$-\,\alpha_\ell(hA) \geq 0, \qquad 0 \leq \ell \leq k-1. \tag{10}$$

We next give the main result of the paper.

Theorem 2. *The order of a positive exponential k-step method is two at most.*

Proof. Our main tools for the proof of Theorem 2 are the representation (7b) of the coefficient functions as Laplace-Stieltjes transforms and further the characterisation of positivity given in Section 2. For the following, we set $a_\ell(t) = 0 = b_\ell(t)$ for $t \leq 0$. We note that due to Corollary 1, it is justified to work with the complex variable z instead of the linear operator hA. For the characteristic function of the interval $[r,s)$, we henceforth employ the abbreviation

$$Y_{[r,s)}(t) = \begin{cases} 1 & \text{if } r \leq t < s, \\ 0 & \text{else.} \end{cases}$$

(i) We first show that the validity of the first order condition (9a) together with the requirement (10) imply that the coefficient functions α_ℓ are of the form

$$\alpha_\ell(z) = -\,\mu_{k-\ell}\,\mathrm{e}^{(k-\ell)z}, \qquad \mu_{k-\ell} \geq 0, \qquad 0 \leq \ell \leq k-1, \tag{11}$$

or, equivalently, that the associated functions a_ℓ are given by

$$a_\ell(t) = -\,\mu_{k-\ell}\,Y_{[k-\ell,\infty)}(t), \qquad \mu_{k-\ell} \geq 0, \qquad 0 \leq \ell \leq k-1. \tag{12}$$

Inserting (7b) into (9a) and applying $\alpha_k(z) = 1$, we get

$$\mathrm{e}^{kz} = -\sum_{\ell=0}^{k-1} \alpha_\ell(z)\,\mathrm{e}^{\ell z} = -\sum_{\ell=0}^{k-1} \int_0^\infty \mathrm{e}^{tz}\,Y_{[\ell,\infty)}(t)\,\mathrm{d}a_\ell(t-\ell)$$

and furthermore conclude

$$Y_{[k,\infty)}(t) = -\sum_{\ell=0}^{k-1} a_\ell(t-\ell)\,Y_{[\ell,\infty)}(t). \tag{13}$$

From (10) and Remark 1 we deduce that the function $-\,\alpha_\ell$ is absolutely monotonic and thus Theorem 1 shows that $-\,a_\ell$ is non-decreasing. Due to the fact that $a_\ell(0) = 0$, we finally obtain (12). For the following considerations, accordingly to our choice $\alpha_k(z) = 1$, it is useful to define $\mu_0 = -\,1$. As a consequence, inserting (11) into (9a) we have

$$\sum_{\ell=1}^{k} \mu_\ell = -\,\mu_0 = 1. \tag{14}$$

(ii) We next reformulate the order conditions in terms of the functions a_ℓ and b_ℓ given by (7b). Inserting (11) into (9b), we have

$$-\sum_{\ell=1}^{k} \mu_{k-\ell}\, \ell^q\, \mathrm{e}^{(k-\ell)z}\, \varphi_q(\ell z) = \sum_{\ell=0}^{k} \beta_\ell(z) \frac{\ell^{q-1}}{(q-1)!}, \qquad 1 \le q \le p.$$

For the following considerations, it is convenient to employ the abbreviation

$$\chi_{q;k-\ell,k}(t) = \frac{\ell^q - (k-t)^q}{q}\, Y_{[k-\ell,k)}(t) + \frac{\ell^q}{q}\, Y_{[k,\infty)}(t), \tag{15}$$

Obviously, $\chi_{q;k-\ell,k}$ is a continuous function such that the support of its derivative is contained in the interval $[k-\ell, k)$. Therefore, making use of the fact that

$$\mathrm{e}^{(k-\ell)z}\, \varphi_q(\ell z) = \frac{1}{\ell^q} \int_0^\infty \mathrm{e}^{tz}\, \frac{(k-t)^{q-1}}{(q-1)!}\, Y_{[k-\ell,k)}(t)\; \mathrm{d}t,$$

see (6) for the definition of φ_q, we obtain

$$-\sum_{\ell=1}^{k} \mu_{k-\ell}\, \chi_{q;k-\ell,k}(t) = \sum_{\ell=0}^{k} \ell^{q-1} b_\ell(t), \qquad 1 \le q \le p. \tag{16}$$

(iii) Exploiting the relations given above, we now show that the assumption $p \ge 3$ and the requirement of positivity, that is, the assumptions $\mu_\ell \ge 0$ for $1 \le \ell \le k$ and $b_\ell(t)$ a non-decreasing function for any $t \in \mathbb{R}$ and $0 \le \ell \le k$, lead to a contradiction. We recall that by definition $\mu_0 = -1$. Regarding the order conditions (16), restricting t to the first interval $[0,1)$, we obtain the following relations for the derivatives[2]

$$\sum_{\ell=0}^{k} b'_\ell(t) = 1, \qquad \sum_{\ell=0}^{k} \ell\, b'_\ell(t) = k - t, \qquad \sum_{\ell=0}^{k} \ell^2\, b'_\ell(t) = (k-t)^2. \tag{17}$$

Taking a suitable linear combination of (17), it follows

$$\sum_{\ell=0}^{k} (t-k+\ell)^2\, b'_\ell(t) = 0.$$

Using that the functions b'_ℓ are non-negative, we conclude that they vanish on $[0,1)$. This contradicts the first relation in (17). □

[2] As the function b_ℓ is non-decreasing, its derivative exists almost everywhere and is non-negative. Assertions involving b'_ℓ are thus valid for almost all t.

Remark 2. The order two barrier of Theorem 2 is sharp in the sense that there exist positive second-order schemes. A simple example is given by the exponential trapezoidal rule where $k = 1$, $\alpha_0(z) = -\mathrm{e}^z$, $\alpha_1 = 1$, $\beta_0 = \varphi_1 - \varphi_2$, and $\beta_1 = \varphi_2$.

For *analytic* semigroups it is well-known that the order conditions (9b) can be weakened, see e.g. [9]. Following the lines of [10] it can be shown that an order two barrier holds in this case, too. For instance, the exponential midpoint rule with $k = 2$, $\alpha_0(z) = -\mathrm{e}^{2z}$, $\alpha_1 = 0$, $\alpha_2 = 1$, $\beta_1(z) = 2\,\varphi_1(2z)$, and $\beta_0 = \beta_2 = 0$ has weak order two and preserves positivity.

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