ON A MULTISTEP METHOD APPROXIMATING A LINEAR SECTORIAL EVOLUTION EQUATION

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Abstract. This paper concerns the linear multistep approximation of an abstract dissipative linear sectorial evolution equation on a Banach space X. We study how well the semigroup generated by a sectorial operator A is approximated by the numerical semigroup generated by a q-step, strictly $A(\alpha)$-stable multistep method. An error bound of the same order of the applied method is obtained.

Key words. Sectorial operator, multistep methods, semigroup

1 Introduction

Many problems encountered in applications, e.g. the linear and nonlinear heat equation, nuclear reaction dynamics, aircraft and ship design, population genetics, the Navier-Stokes equation or other convection-diffusion equations ([1], [2], [16]) can be modelled in the abstract form

$$u_t + Au = f(t,u), \qquad t \geq 0, \tag{1}$$

where A is a sectorial operator on a Banach space X. Equations of type (1), known as *sectorial evolution equations*, and the properties of the operator A have been deeply studied in [10], [16] and [26] and theoretical results of existence and uniqueness of solution for (1) are known if the function f satisfies certain continuity properties. Moreover, in recent years there has been a great interest in the numerical approximation of (1) and of its asymptotic structures and invariant sets (see [3], [14], [15], [17], [27]).
In this paper we address the simpler linear equation

$$u_t + Au = 0, \qquad t > 0, \tag{2}$$

and the approximation in time of e^{-At}, the analytic semigroup generated by the operator A. This approximation is performed by a q-step linear multistep method

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and has been previously considered in [4], [9], [22], and more recently in [25] and [17]. A first order error estimate for the multistep approximation of (2) is also provided in [17] and used respectively there and in [27] to prove the existence and convergence of local attractors and inertial manifolds for a multistep method discretising (1).
Here, using the same approach as [17] in constructing the numerical semigroup approximating e^{-At}, we improve the known linear order error between the real and the numerical semigroup and we obtain an error estimate of high order.
This paper is organised as follows. In Section 2 we give a formal definition of a sectorial operator and we introduce our problem, we recall those concepts on linear multistep methods needed to develop our results and we consider the linear multistep approximation of (2). In Section 3 we highlight the difficulties encountered in this approximation and we provide the tools for solving them. The technique developed in Section 3 will be applied in Section 4 for proving our principal error estimate. Finally, we will briefly discuss the possible application of the error estimate to nonlinear problems, as well as its technical restrictions.

2 Sectorial equation and multistep method

Let X be a complex Banach space and $D(A)$ be a subspace of X.

Definition 1 *A closed, densely defined operator $A : D(A) \to X$ is called* **sectorial operator** *if there exist two constants $a \in \mathbb{R}$ and $M \geq 1$ and an angle $\theta \in (0, \frac{\pi}{2})$ such that*

$$\|(zI - A)^{-1}\| \leq \frac{M}{|z-a|} \qquad \text{for all } z \in \mathbb{C} \setminus S_{a,\theta}, \tag{3}$$

where the sector $S_{a,\theta} = \{z \in \mathbb{C} \setminus \{a\} : |\arg(z-a)| \leq \theta\}$ contains the spectrum of the operator A.

Given a sectorial operator A we consider the dissipative linear equation:

$$u_t + Au = 0, \qquad t > 0, \qquad u(0) = u_0 \in X, \tag{4}$$

whose solution can be written as $u(t) = e^{-At}u_0$, where e^{-At} is the bounded, analytic semigroup generated by A (see [10], [16], [26]). To approximate (4) in time we consider a multistep method. Before starting our approximation we recall some known definition and properties of a multistep methods.
Consider a general equation $u_t = F(t, u)$. A *q-step linear multistep method*, for approximating the solution of this equation is given from the formula

$$\sum_{i=0}^{q} \alpha_i U^{n+i} = h \sum_{i=0}^{q} \beta_i F((n+i)h, U^{n+i}), \qquad \text{for all } n \geq 0, \tag{5}$$

where h is the time-step size and each U^{n+q} is an approximation of the exact solution $u(t_{n+q})$, at the instant $t_{n+q} = (n+q)h$. We will assume that the starting values

$\{U^i\}_{i=0}^{q-1}$ are given and that $\{\alpha_i\}_{i=0}^{q}$ and $\{\beta_i\}_{i=0}^{q}$ are real constants, with α_0 and β_0 not both being zero and normalised so that $\alpha_q = 1$. These constants define the particular method; if $\beta_q = 0$ the method is *explicit*, and it is *implicit* otherwise. In term of the parameters α_i and β_i the *characteristic polynomials* of the method are

$$\rho(w) = \sum_{i=0}^{q} \alpha_i w^i, \qquad \sigma(w) = \sum_{i=0}^{q} \beta_i w^i.$$

The multistep method is said to be *irreducible* if $\rho(w)$ and $\sigma(w)$ have no common factors, and *reducible* otherwise. Sometimes the multistep method is also called $(\rho, sigma)$ method.

Definition 2 *For the q-step linear multistep method (5), we define*

$$\delta_i(z) = \frac{\alpha_i + \beta_i z}{\alpha_q + \beta_q z}, \qquad for\ i = 0, 1, \ldots, q-1,$$

and the **companion matrix** *of the method*

$$T(z) = \left[\begin{array}{c|cccc} 0 & 1 & & & \\ \vdots & & & \ddots & \\ 0 & & & & 1 \\ \hline -\delta_0(z) & -\delta_1(z) & & \ldots & -\delta_{q-1}(z) \end{array}\right]. \tag{6}$$

It is known that the eigenvalues of $T(z)$ are the w-roots of the equation $P(w; z) = \rho(w) + z\sigma(w) = 0$, and that when $z \to \infty$ these roots will tend to those of the polynomial $\sigma(w)$ (see [12]). Moreover, the polynomial $P(w; z)$ is an analytic function mapping $\mathbb{C}^2$ into $\mathbb{C}$.
The multistep method (5) is of order $p \geq 1$ if

$$\sum_{i=0}^{q} \alpha_i = 0 \qquad \text{and} \qquad \sum_{i=0}^{q} \alpha_i i^k = k \sum_{i=0}^{q} \beta_i i^{k-1} \qquad \text{for } k = 1, \ldots, p.$$

or equivalently (see [12])

$$\rho(e^z) - z\sigma(e^z) = \mathcal{O}(z^{p+1}). \tag{7}$$

Definition 3 *The linear multistep method (5) is said to be* **strictly** $\boldsymbol{A(\alpha)}$**-stable***, for some* $\alpha \in [0, \frac{\pi}{2})$*, if the spectrum of its companion matrix* $T(z)$*,* $\sigma(T(z)) = \{\lambda_1(z), \ldots, \lambda_q(z)\}$*, ordered in non-increasing magnitude* $|\lambda_1(z)| \geq |\lambda_2(z)| \geq \ldots \geq |\lambda_q(z)|$*, satisfies:*

$$|\lambda_1(z)| < 1 \qquad for\ all\ z \in \Sigma_\alpha \backslash \{0\}; \quad |\lambda_1(0)| = 1, \tag{8}$$

$$|\lambda_i(z)| < 1 \qquad for\ i = 2, \ldots, q, \quad for\ all\ z \in \Sigma_\alpha, \tag{9}$$

where $\Sigma_\alpha := \{z \in \mathbb{C} \backslash \{0\} : |\arg(-z)| \leq \alpha\} \cup \{0\}$.

Assumptions Henceforth, we shall assume that $u_t + Au = 0$ is approximated by a q-step, pth-order, irreducible, strictly $A(\alpha)$-stable, linear multistep method with $p, q \geq 1$ and $\alpha \in [\theta, \frac{\pi}{2})$, where θ is the sectorial angle of the operator A.

Applying the multistep method (5) to the equation (4), we obtain

$$\sum_{i=0}^{q} \alpha_i U^{n+i} = -h \sum_{i=0}^{q} \beta_i A U^{n+i}, \qquad \text{for all } n \geq 0, \tag{10}$$

which can be written as

$$(\alpha_q + h\beta_q A)U^{n+q} = -[(\alpha_0, \dots, \alpha_{q-1}) + hA(\beta_0, \dots, \beta_{q-1})]^T \cdot (U^n, \dots, U^{n+q-1}). \tag{11}$$

Consider the linear operator

$$T(hA) = \left[\begin{array}{c|ccc} 0 & I & & \\ \vdots & & \ddots & \\ 0 & & & I \\ \hline -\delta_0(hA) & -\delta_1(hA) & \dots & -\delta_{q-1}(hA) \end{array}\right],$$

where $T(z) \in \mathcal{L}(\mathbb{C}^q)$ is the companion matrix (6), together with the vectors in X^q of the approximate and initial solutions:

$$\mathbf{U}^n = \begin{bmatrix} U^n \\ \vdots \\ U^{n+q-1} \end{bmatrix}, \qquad n \geq 1, \qquad \mathbf{U}^0 = \begin{bmatrix} U^0 \\ \vdots \\ U^{q-1} \end{bmatrix}.$$

Then (11) implies that $\mathbf{U}^{n+1} = T(hA)\mathbf{U}^n$, and hence $\mathbf{U}^n = T^n(hA)\mathbf{U}^0$.

The family of linear operators $\{T^n(hA)\}_{n \geq 0}$ defines a discrete semigroup on X^q. To show that this numerical semigroup approximates in some sense the real semigroup e^{-At} and so the solution of (4) we need to overcome the problem of commensurability which appears when $q > 1$, since in this case these two semigroups are defined on different spaces. Conventionally, when a multistep method is used to approximate a single trajectory for a given u_0, that is $e^{-At}u_0$, the mapping defined by the numerical method is described by $y^T T^n(h\ \cdot)v : X \to X$, where $v : X \to X^q$ is the starting method, which is normally a complicated function mapping the initial data $u_0 \in X$ to an approximation of the vector $[u_0, e^{-hA}u_0, \dots, e^{-(q-1)hA}u_0]$, while $y^T : X^q \to X$ is the finishing method, which is usually the projection onto the last coordinate. However, for any choice of v and y^T, the previous function cannot represent a semigroup unless $y^T T^n(h\ \cdot)v y^T T^m(h\ \cdot)v = y^T T^{n+m}(h\ \cdot)v$ for all $n, m \geq 0$. In order for this to be true y^T and v must satisfy a rather complicated condition involving all the left and right eigenvectors of $T^n(z)$, making it unlikely to be satisfied for common linear multistep methods. Hence, rather than modifying the numerical semigroup to act on X, we modify the real semigroup e^{-At} to act on X^q.

To do this we consider the largest eigenvalue in magnitude (*principal eigenvalue*) of $T(z)$, say $\lambda_1(z)$, and denoting by $y^T(z)$ and $v(z)$ the associated left and right eigenvectors, normalised so that

$$y^T(z)v(z) = 1, \tag{12}$$

we consider the operator

$$ve^{-At}y^T : X^q \to X^q. \tag{13}$$

Observe that the family $\{ve^{-At}y^T\}_{t\geq 0}$ is not a conventional semigroup on X^q because $v(0)y^T(0)$ is not the identity on X^q; nevertheless the theory of semigroups that does not require the first axiom of the semigroup is valid for these operators and we will continue to call it semigroup.

3 Study of the numerical semigroup

Having introduced the modified semigroup $ve^{-At}y^T$ and the numerical semigroup $T^n(hA)$, our aim is to find necessary conditions to ensure a good estimate for the approximation error:

$$\|T^n(hA) - v(hA)e^{-At}y^T(hA)\|_{\mathcal{L}(X^q)}. \tag{14}$$

To bound (14) we will study the behaviour of $T(z)$, and therefore of its principal eigenvectors $v(z)$ and $y^T(z)$, for all $z \in \overline{S}_{0,\theta} = \{z \in \mathbb{C} \setminus \{0\} \; : |\arg(z)| \leq \theta\}$. We will find conditions on (ρ, σ) method ensuring that $\lambda_1(z)$ is analytic thoughout $S_{0,\theta}$. Under these circumstances, y^T and v may also be analytically defined and maybe renormalised as in (12), for $z \in S_{0,\theta}$. As we will see, when $\lambda_1(z)$ is not simple, $y^T(z)$ and $v(z)$ are orthogonal and we cannot renormalise their scalar product. Difficulties also arise close to a point where $\lambda_1(z)$ is not simple. In this connection, we recall that the quantity

$$s(\lambda_1(z)) = |y^T(z)v(z)|$$

is known as the *condition number* of the eigenvalue $\lambda_1(z)$ (see [11]). Generally speaking, if one makes a perturbation of order ε to the matrix $T(z)$, then its eigenvalue $\lambda_1(z)$ will be perturbed by $\varepsilon/s(\lambda_1(z))$ and so if $s(\lambda_1(z))$ is very small $\lambda_1(z)$ is regarded as ill-conditioned. Thus, near to a point where $y^T(z)$ and $v(z)$ are orthogonal, the principal eigenvalue will be ill-conditioned.

We start the analysis of the principal eigenvalue and eigenvectors of $T(z)$ recalling a known result about their behaviour in a neighbourhood of the origin.

Lemma 1 (Hill-Süli). *There exists a neighbourhood N_0 of the origin such that $\lambda_1(z)$, the principal eigenvalue of $T(z)$, is an analytic function with*

$$\lambda_1(z) - e^{-z} = \mathcal{O}(z^{p+1}), \qquad z \in N_0. \tag{15}$$

Furthermore, the corresponding left and right eigenvectors $y^T(z)$ and $v(z)$ may be analytically defined in N_0, so that $v(z) = [1, \lambda_1(z), \ldots, \lambda_1(z)^{q-1}]^T$ and $y^T(z)v(z) = 1$.

Proof. See [17] Lemma 2.1. $\square$

We start to study the behaviour of $\lambda_1(z)$ and of its eigenvectors in a region $\overline{S}_{0,\theta}\backslash N_0$.

Lemma 2 *Let N_0 be the neighbourhood of the origin as in Lemma 1. Then for all $z \in \overline{S}_{0,\theta}\backslash N_0$ such that $\lambda_1(z_0) \neq 0$ is a simple eigenvalue of $T(z)$, there exists a neighbourhood $N(z_0)$ of z_0 such that $\lambda_1(z)$ is an analytic function of z, for all $z \in N(z_0)$. Moreover, the corresponding left and right eigenvectors $y^T(z)$ and $v(z)$ may be analytically defined in $N(z_0)$, so that $v(z) = [1, \lambda_1(z), \ldots, \lambda_1(z)^{q-1}]^T$ and $y^T(z)v(z) \neq 0$.*

Proof. Let $z_0 \in S_{0,\theta}\backslash N_0$, where N_0 is a neighbourhood of the origin as in Lemma 1 and suppose $\lambda_1(z_0) \neq 0$ is a simple root of $P(w; z)$. Then $P(\lambda_1(z_0); z_0) = 0$ and $\frac{\partial P}{\partial w}(\lambda_1(z_0); z_0) \neq 0$. The analytic implicit function theorem implies the existence of a neighbourhood $N(z_0)$ of the point z_0 in which $\lambda_1(z)$ is a simple root of $P(w; z)$. Moreover, because $P(w; z)$ is analytic, the function $\lambda_1(z)$ is analytic for every $z \in N(z_0)$. Suppose $v(z_0), y^T(z_0)$ are the associated right and the left eigenvectors at z_0. The form of the right eigenvalue $v(z_0)$ may be verified by direct substitution, while the individual components of $y^T(z_0)$ satisfy

$$
\begin{aligned}
&-\delta_0(z_0)y_q(z_0) = \lambda_1(z_0)y_1(z_0)\\
&y_i(z_0) - \delta_i(z_0)y_q(z_0) = \lambda_i(z_0)y_{i+1}(z_0) \qquad \text{for } i = 1, \ldots, q-1.
\end{aligned}
\tag{16}
$$

Since $y_q(z_0) = 0$ implies $y_i(z_0) = 0$ for all i, we conclude that $y_q(z_0) \neq 0$. Thus by equations (16) all components of $y^T(z_0)$ can be written as

$$
y_i(z_0) = -\frac{y_q(z_0)}{\lambda_1(z_0)^i}\sum_{k=0}^{i-1}\delta_k(z_0)\lambda_1(z_0)^k, \qquad i = 1, \ldots, q-1.
$$

At $z = z_0$ consider

$$
\begin{aligned}
y^T(z_0)v(z_0) &= \sum_{i=1}^{q} y_i(z_0)v_i(z_0)\\
&= y_q(z_0)\lambda_1(z_0)^{q-1} - \frac{1}{\lambda_1(z_0)}\left(\sum_{i=1}^{q-1}\sum_{k=0}^{i-1}\delta_k(z_0)\lambda_1(z_0)^k\right)y_q(z_0)\\
&= y_q(z_0)\lambda_1(z_0)^{q-1} - \frac{1}{\lambda_1(z_0)}\left[(q-1)\delta_0(z_0) + (q-2)\delta_1(z_0)\lambda_1(z_0)\right.\\
&\quad \left. + \big(q-3)\delta_2(z_0)\lambda_1(z_0)^2 + \ldots + \delta_{q-2}(z_0)\lambda_1(z_0)^{q-2}\right] y_q(z_0).
\end{aligned}
\tag{17}
$$

By the chain rule and the product rule result

$$\begin{aligned}\frac{1}{\alpha_q + z\beta_q}\left[\frac{\partial P(w;z)}{\partial w} w - (q-1)P(w;z)\right] = \\ -(q-1)\delta_0(z) - (q-2)\delta_1(z)w - \ldots - \delta_{q-2}(z)w^{q-2} + w^q.\end{aligned} \tag{18}$$

Thus evaluating (18) at $(z_0, \lambda_1(z_0))$, and applying (17),

$$y^T(z_0)v(z_0) = \frac{y_q(z_0)}{\lambda_1(z_0)}\frac{1}{\alpha_q + z_0\beta_q}\left[\frac{\partial P(\lambda_1(z_0);z_0)}{\partial w}\lambda_1(z_0) - (q-1)P(\lambda_1(z_0);z_0)\right]. \tag{19}$$

Since $\lambda_1(z)$ is a simple eigenvalue at $z = z_0$ (19) implies that $y^T(z_0)v(z_0) \neq 0$, and hence by continuity $y^T(z)v(z) \neq 0$ for all $z \in N(z_0)$.
In the same way it can be prove that for $z \to \infty$ there exists an $R > 0$ such that for any $z \in S_{0,\theta} \setminus N_0$, with $|z| > R$, $\lambda_1(z)$ is an analytic function with $y^T(z)$ and $v(z)$ and that $y^T(z)v(z) \neq 0$. □

Observe that when $\lambda_1(z_0)$ is a repeated root of the polynomial $P(w;z)$, with multiplicity $\alpha \geq 2$,

$$\begin{aligned} &P(\lambda_1(z_0);z_0) = \frac{\partial P(\lambda_1(z_0);z_0)}{\partial w} = \ldots = \frac{\partial^{\alpha-1}P(\lambda_1(z_0);z_0)}{\partial w^{\alpha-1}} = 0, \\ &\frac{\partial^{\alpha}P(\lambda_1(z_0);z_0)}{\partial w^{\alpha}} \neq 0.\end{aligned} \tag{20}$$

Hence, equation (19) implies that $y^T(z_0)v(z_0) = 0$ and therefore, we are not able to renormalise $v(z)$ and $y^T(z)$ at this point z_0. Moreover, if $\lambda_1(z_0) = 0$, by the stability conditions imposed, it is an eigenvalue of multiplicity q thus $v(z_0)$ and $y^T(z_0)$ cannot be renormalised. The analysis of the behaviour of $\lambda_1(z)$ and its associated eigenvectors $v(z)$ and $y^T(z)$ does not depend on $\overline{S}_{0,\theta}$ and therefore it is valid for all $z \in \mathbb{C} \setminus N_0$, where N_0 is a neighbourhood of the origin; also by Lemma 1, $y^T(z)v(z) = 1$ for all $z \in N_0$.

The following result concerns with the behaviour of $\lambda_1(z)$ in a neighbourhood of a multiple root point. We will make use of the Taylor expansion of the polynomial $P(w;z)$. We start to prove a technical lemma.

Lemma 3 *If $z_0 \in \mathbb{C}$ is such that $\lambda_1(z_0)$ is a repeated root of $P(w;z)$, with multiplicity $\alpha \geq 2$, then $\dfrac{\partial P(\lambda_1(z_0);z_0)}{\partial z} \neq 0$.*

Proof. Let $z_0 \in \mathbb{C}$ be such that $\lambda_1(z_0)$ is a repeated root of the polynomial $P(w;z)$ with multiplicity $\alpha \geq 2$. Then, the partial derivatives of $P(w;z)$ with respect to w, evaluated at the point $(z_0, \lambda_1(z_0))$, satisfy

$$P(\lambda_1(z_0); z_0) = \rho(\lambda_1(z_0)) + z_0\sigma(\lambda_1(z_0)) = 0, \tag{21}$$

$$\frac{\partial P(\lambda_1(z_0); z_0)}{\partial w} = \ldots = \frac{\partial^{\alpha-1} P(\lambda_1(z_0); z_0)}{\partial w^{\alpha-1}} = 0, \tag{22}$$

$$\frac{\partial^{\alpha} P(\lambda_1(z_0); z_0)}{\partial w^{\alpha}} \neq 0. \tag{23}$$

We prove the statement by contradiction. Suppose that $\frac{\partial P(\lambda_1(z_0);z_0)}{\partial z} = 0$. Observe that, $\frac{\partial P(w;z)}{\partial z} = \sigma(w)$ and hence, by hypothesis at $z = z_0$, $\sigma(\lambda_1(z_0)) = 0$. This implies that $\lambda_1(z_0)$ is a root of the polynomial $\sigma(w)$. Because of the multiplicity of $\lambda_1(z_0)$, by (21) we deduce that $\rho(\lambda_1(z_0)) = 0$. This implies that $\lambda_1(z_0)$ is also a root of the polynomial $\rho(w)$, which contradicts the irreducibility of the multistep method. This contradiction proves the theorem. □

Theorem 4 *Let $z_0 \in \mathbb{C}$ such that $\lambda_1(z_0)$ is a repeated root of $P(w; z)$ with multiplicity $\alpha \geq 2$. Then there exists a neighbourhood K of z_0, such that for any $z \in K$, the polynomial $P(w; z)$ has simple roots.*

Proof. Let $z \in K_1 \setminus \{z_0\}$, where K_1 is some compact neighbourhood of z_0 and suppose that $w(z)$ is a root of $P(w; z) = 0$. By the Taylor expansion of $P(w; z)$ in a neighbourhood of the repeated root in which henceforth all partial derivatives are evaluated in $(\lambda_1(z_0), z_0)$, we obtain

$$\frac{\partial P}{\partial z}(z - z_0) + \frac{1}{\alpha!}\frac{\partial^{\alpha} P}{\partial w^{\alpha}}(w - \lambda_1(z_0))^{\alpha} + \left(\sum_{i=2}^{\alpha} c_i \frac{\partial^{i} P}{\partial w^{i-1}\partial z}(z - z_0)(w - \lambda_1(z_0))^{i-1}\right) + E_{\alpha+1} = 0, \tag{24}$$

where $c_i = \begin{pmatrix} \alpha \\ i \end{pmatrix}$, $E_{\alpha+1}$ is the error of the Taylor expansion such that

$$|E_{\alpha+1}| \leq C\left(|z - z_0||w - \lambda_1(z_0)|^{\alpha} + |w - \lambda_1(z_0)|^{\alpha+1}\right), \tag{25}$$

where C denote a generic positive constant. Since, by Weierstrass' Theorem, all derivatives of $P(w; z)$ are bounded in any compact set,

$$\left|\frac{\partial P}{\partial z}(z - z_0) + \frac{1}{\alpha!}\frac{\partial^{\alpha} P}{\partial w^{\alpha}}(w - \lambda_1(z_0))^{\alpha}\right| \leq \left(\sum_{i=1}^{\alpha} C|z - z_0||w - \lambda_1(z_0)|^{i}\right) + C|w - \lambda_1(z_0)|^{\alpha+1}.$$

Dividing both sides by $|z - z_0|$,

$$\left|\frac{\partial P}{\partial z} + \frac{1}{\alpha!}\frac{\partial^{\alpha} P}{\partial w^{\alpha}}\frac{(w - \lambda_1(z_0))^{\alpha}}{z - z_0}\right| \leq \left(\sum_{i=1}^{\alpha} C|w - \lambda_1(z_0)|^{i}\right) + C\frac{|w - \lambda_1(z_0)|^{\alpha}}{|z - z_0|}|w - \lambda_1(z_0)|. \tag{26}$$

Since $\dfrac{\partial P(\lambda_1(z_0); z_0)}{\partial z} \neq 0$ and $w(\cdot)$ is a continuous function as it is a root of an analytic polynomial, (26) implies

$$\lim_{z \to z_0} \frac{\partial^\alpha P}{\partial w^\alpha} \frac{(w - \lambda_1(z_0))^\alpha}{z - z_0} = -(\alpha!) \frac{\partial P(\lambda_1(z_0); z_0)}{\partial z}. \tag{27}$$

By contradiction, suppose that there is no neighbourhood K of z_0 as in the statement of the theorem and so let $w(z)$ also be a root of $\frac{\partial P(w;z)}{\partial w}$. Using the Taylor expansion of $\frac{\partial P(w;z)}{\partial w}$ we deduce that

$$\frac{\partial^2 P}{\partial z \partial w}(z - z_0) + \left(\sum_{i=3}^{\alpha} c_i^* \frac{\partial^i P}{\partial w^{i-1} \partial z}(z - z_0)(w - \lambda_1(z_0))^{i-2} \right)$$

$$+ \frac{1}{(\alpha - 1)!} \frac{\partial^\alpha P}{\partial w^\alpha}(w - \lambda_1(z_0))^{\alpha - 1} + \hat{E}_\alpha = 0,$$

where all the derivatives are evaluated at $(\lambda_1(z_0), z_0)$, c_i^*, for $i = 3, \ldots, \alpha$ are constants and $\hat{E}_\alpha$ is the error of the Taylor expansion such that

$$|\hat{E}_\alpha| \leq C \left(|z - z_0||w - \lambda_1(z_0)|^{\alpha-1} + |w - \lambda_1(z_0)|^\alpha \right).$$

By Weierstrass' theorem

$$\left| \frac{\partial^2 P}{\partial z \partial w}(z - z_0) + \frac{1}{(\alpha - 1)!} \frac{\partial^\alpha P}{\partial w^\alpha}(w - \lambda_1(z_0))^{\alpha-1} \right| \leq$$

$$\leq \left(\sum_{k=1}^{\alpha-2} C|z - z_0||w - \lambda_1(z_0)|^k \right) + C|z - z_0||w - \lambda_1(z_0)|^{\alpha-1} + C|w - \lambda_1(z_0)|^\alpha,$$

with C positive constant. Multiplying by the factor $\dfrac{|w - \lambda_1(z_0)|}{|z - z_0|}$, we deduce

$$\left| \frac{\partial^2 P}{\partial z \partial w}(w - \lambda_1(z)) + \frac{1}{(\alpha - 1)!} \frac{\partial^\alpha P}{\partial w^\alpha} \frac{(w - \lambda_1(z_0))^\alpha}{z - z_0} \right| \leq$$

$$\leq \left(\sum_{j=2}^{\alpha} C|w - \lambda_1(z_0)|^j \right) + C \frac{|w - \lambda_1(z_0)|^\alpha}{|z - z_0|} |w - \lambda_1(z_0)|. \tag{28}$$

As $z \to z_0$ (28) and (27) imply that $\dfrac{\partial P(\lambda_1(z_0); z_0)}{\partial z} = 0$, which contradicts our assumption. This contradiction proves the theorem. □

Analogously we have

Theorem 5 *Let $\mu = \lim_{z \to \infty} \lambda_1(z)$ be an eigenvalue of $T(\infty)$ of multiplicity $\alpha \geq 2$. Then there exists $R > 0$ such that for any $z \in \mathbb{C} \setminus B(0, R)$, $\lambda_1(z)$ is a simple root.*

Proof. The theorem may be proved in the same fashion of the previous theorem. □

Theorem 6 *There exists at most a finite number of $z_i \in \mathbb{C}$ such that $\lambda_1(z_i)$ is a multiple root of the polynomial $P(w; z)$.*

Proof. The proof is made by contradiction. Suppose that there exists an infinite number of points $z_n \in \mathbb{C}$, $n \in \mathbb{N}$, such that in each of these points $\lambda_1(z)$ is a multiple root of $P(w; z)$. By Theorem 5 then there exists $R > 0$ such that if $\lambda_1(z_n)$ is a multiple root $z_n \in \overline{B}(0, R)$, for $n \in \mathbb{N}$.
Note that $\overline{B}(0, R)$ is a compact set, and so by Bolzano-Weierstrass' theorem there exists a $z^* \in \mathbb{C}$ limit point of the infinite sequence z_n. By continuity of $P(w; z)$ and $\lambda_1(z)$, we deduce

$$\lim_{n\to\infty} P(\lambda_1(z_n); z_n) = P(\lambda_1(z^*); z^*) = 0.$$

Similarly,

$$\lim_{n\to\infty} \frac{\partial P(\lambda_1(z_n); z_n)}{\partial w} = \frac{\partial P(\lambda_1(z^*); z^*)}{\partial w} = 0.$$

Hence, $\lambda_1(z^*)$ is a multiple root of $P(w; z)$. Since $z_n \to z^*$, this contradicts Theorem 4 and hence, Theorem 6 is true. □

Having solved the problem about the existence of the modified semigroup for all points at which $\lambda_1(z)$ is a single eigenvalue of $T(z)$, we study the behaviour of $T^n(z)$ to obtain information about the order of accuracy of the method. The following lemma establish some properties of the approximation in a region of the complex plane associated with a contour integral appearing later.

Lemma 7 *There exists a neighbourhood N_0 of the origin, and constants $C > 0$ and $\Lambda \in (0, 1)$, such that*

$$\|T^n(z) - v(z)e^{-nz}y^T(z)\| \le C(\Lambda^n + |z^p e^{-nz}|), \tag{29}$$

for all $z \in N_0 \cap (\overline{B}(0, (\operatorname{cosec}\,\theta)/n) \cup \overline{S}_{0,\theta})$ and all $n \in \mathbb{N}$.

Proof. We follow a technique similar to that used by Hill and Süli [17]. Let N_0 be as in the statement of Lemma 1. For $z \in N_0$ and $n \in \mathbb{N}$

$$\begin{aligned}
&\|T^n(z) - v(z)e^{-nz}y^T(z)\| \\
&= \|T^n(z) - v(z)\lambda_1(z)^n y^T(z) + v(z)\lambda_1(z)^n y^T(z) - v(z)e^{-nz}y^T(z)\| \\
&\le \|T^n(z) - v(z)\lambda_1(z)^n y^T(z)\| + |\lambda_1(z)^n - e^{-nz}|\|v(z)y^T(z)\| \\
&= I_1 + I_2.
\end{aligned}$$

Consider the matrix $(T(z) - v(z)\lambda_1(z)y^T(z)) \in \mathcal{L}(\mathbb{C}^q)$. It has eigenvalues

$$\{0, \lambda_2(z), \ldots, \lambda_q(z)\}.$$

Using the construction of Isaacson and Keller ([21], Chapter 1, Theorems 1 and 3), for any square matrix M of order q and any arbitrary $\varepsilon > 0$, there exists a non singular matrix $P \in \mathcal{L}(\mathbb{C}^q)$, such that $\|P^{-1}MP\| \leq \rho(M) + \varepsilon$, where $\rho(M)$ denotes the spectral radius of M. So since $\rho(T(z) - v(z)\lambda_1(z)y^T(z)) = |\lambda_2(z)| < 1$, there exist non singular matrices $P(z)$ and $P^{-1}(z)$, in a neighbourhood of the origin, continuously dependent on z, such that

$$\| \left(P^{-1}(z)(T(z) - v(z)\lambda_1(z)y^T(z))P(z)\right)^n \| \leq \left(\frac{|\lambda_2(z)| + 1}{2}\right)^n.$$

Because $y^T(z)$ and $v(z)$ are the left and right eigenvalues of $\lambda_1(z)$ and they verify $y^T(z)v(z) = 1$, we deduce the identity

$$\left(T(z) - v(z)\lambda_1(z)y^T(z)\right)^n = T(z)^n - v(z)\lambda_1^n(z)y^T(z).$$

Finally,

$$\begin{aligned} I_1 &= \|(T(z) - v(z)\lambda_1(z)y^T(z))^n\| \\ &\leq \|P(z)\|\|P^{-1}(z)(T(z) - v(z)\lambda_1(z)y^T(z))^n P(z)\|\|P^{-1}(z)\| \\ &\leq C(z)\left(\frac{|\lambda_2(z)| + 1}{2}\right)^n. \end{aligned} \tag{30}$$

The functions $C(z)$ and $((|\lambda_2(z)| + 1)/2)$ may be uniformly bounded in N_0 by constants $C > 0$ and $\Lambda \in (0, 1)$, respectively, in which case,

$$I_1 \leq C\Lambda^n, \qquad \text{for all } z \in N_0 \text{ and } n \in \mathbb{N}. \tag{31}$$

Now we consider $|\lambda_1^n(z) - e^{-nz}|$ in N_0. By Lemma 1,

$$\lambda_1(z) = e^{-z} + C(z)z^{p+1},$$

for some analytic function $C(z)$ and $z \in N_0$. This implies

$$\log(\lambda_1(z)) = -z + C_1(z)z^{p+1},$$

for some analytic function $C_1(z)$ in a possibly refined neighbourhood N_0. Therefore,

$$\lambda_1(z)^n = e^{n\log(\lambda_1(z))} = e^{-nz}\exp(nC_1(z)z^{p+1}).$$

Hence,

$$\begin{aligned} |\lambda_1^n(z) - e^{-nz}| &\leq |e^{-nz}||\exp(nC_1(z)z^{p+1}) - 1| \\ &\leq A(z)B(z)|z^p e^{-nz}|, \end{aligned}$$

where

$$A(z) = \left| \frac{\exp(nC_1(z)z^{p+1}) - 1}{nC_1(z)z^{p+1}} \right|, \qquad B(z) = |nC_1(z)z|.$$

Note that the functions $A(z)$ and $B(z)$ may be bounded independently of n in the region $N_0 \cap (\overline{B}(0, (\text{cosec } \theta)/n) \cup \overline{S}_{0,\theta})$, provided $\text{diam}(N_0)$ is sufficiently small and n large enough, so

$$I_2 \leq C|z^p e^{-nz}|. \tag{32}$$

By (31) and (32), the theorem follows. □

Here we recall a result of Le Roux (see [22]), characterising the behaviour of the operator $T^n(z)$ away from a neighbourhood N_0 of the origin.

Lemma 8 *Consider a strictly $A(\alpha)$-stable, linear multistep method (5). There exist positive constants R, μ and C such that*

$$\|T^n(z)\|_{\mathcal{L}(C^q)} \leq Ce^{-\mu n},$$

$$\|T^n(z) - T^n(\infty)\|_{\mathcal{L}(C^q)} \leq \frac{Ce^{-\mu n}}{|z|},$$

for any $z \in \overline{S}_{0,\theta}$ with $|z| \geq R$.

Proof. [22], Lemma 3 and Lemma 4. □

Lemma 9 *Consider a strictly $A(\alpha)$-stable, linear multistep method (5). There exist positive constants R, C and $\Lambda \in (0,1)$, such that*

$$\|T^n(z) - v(z)e^{-nz}y^T(z)\|_{\mathcal{L}(C^q)} \leq C\Lambda^n,$$

for any $z \in \overline{S}_{0,\theta}$ with $|z| \geq R$.

Proof. Let R, μ and C as in the statement of Lemma 8. Consider a $z \in \overline{S}_{0,\theta}$ with $|z| \geq R$. Then $z = |z|e^{\pm i\phi}$, with $0 \leq \phi \leq \theta$

$$\begin{aligned} \|T^n(z) - v(z)e^{-nz}y^T(z)\| &\leq \|T^n(z)\| + |e^{-nz}|\|v(z)y^T(z)\| \leq \\ &\leq Ce^{-\mu n} + C_1 e^{-n|z|\cos\phi} \\ &\leq Ce^{-\mu n} + C_1 e^{-nR\cos\theta}. \end{aligned}$$

Let $\Lambda = \max\{e^{-\mu}, e^{-R\cos\theta}\} \in (0,1)$; it is independent of n and z, thus we deduce that

$$\|T^n(z) - v(z)e^{-nz}y^T(z)\|_{\mathcal{L}(C^q)} \leq C\Lambda^n,$$

and the lemma follows. □

In the sequel $\Lambda \in (0,1)$ will denote the constant Λ in the statement of Lemma 9.

4 Main result

Now we prove our main result when the principal eigenvalue $\lambda_1(z)$ of $T(z)$ is a simple root.

Theorem 10 *Suppose that A is a sectorial operator satisfying Definition 1 with $M \geq 1$, $a \geq 0$ and $\theta \in (0, \pi/2)$. Suppose that the equation $u_t + Au = 0$ is discretised by a pth-order, q-step, linear multistep method, with $p, q \geq 1$, strictly $A(\alpha)$-stable for some $\alpha \in [\theta, \pi/2)$, with companion matrix $T(z)$. Assume, in addition, that $\lambda_1(z)$, the principal eigenvalue of $T(z)$, is simple for all $z \in S_{0,\theta}$ and that its left and right eigenvectors, $y^T(z)$ and $v(z)$ are normalised so that $y^T(z)v(z) = 1$.*
Then, the linear operator $T^n(hA) : X^q \to X^q$ is well defined for all $n \geq 0$ and there exists a constant C_0, independent of n, a, and h, such that for h sufficiently small and n sufficiently large,

$$\|T^n(hA) - v(hA)e^{-nhA}y^T(hA)\|_{\mathcal{L}(X^q)} \leq C_0 e^{-anh}(ah + 1/n)^p, \quad \textit{for all } n \in \mathbb{N}. \tag{33}$$

Proof. Let R be the largest radius such that $B(0, 2R) \subset N_0$, where N_0 is as in the statement of Lemma 1 . Let us choose the maximum of the constant Λ in the previous Remark and $\exp(-(R\cos\theta)/2)$, and denote it again by Λ. For $a > 0$, we require that $h \leq \frac{|\log \Lambda|}{2a}$, (no restriction is necessary if $a = 0$). This implies that $e^{ah}\Lambda \leq \Lambda^{\frac{1}{2}} < 1$.
We consider first the case $n \geq 2/R$. The function $f(z) \equiv T^n(z) - T^n(\infty) - v(z)e^{-nz}y^T(z)$ is analytic in the region $\overline{S}_{0,\theta} \cup N_0$ and vanishes at ∞. Using the Dunford-Taylor integral formulation ([8], Section VII.9), for any operator B,

$$f(B) = f(\infty)I + \frac{1}{2\pi i}\int_\Gamma f(z)R(z; B)dz, \tag{34}$$

where Γ consists of a finite number of Jordan arcs lying in a region in which $f(z)$ is analytic. In particular consider (34 for the operator $B = hA$,

$$\begin{aligned} &e^{anh}\left(T^n(hA) - v(hA)e^{-nhA}y^T(hA)\right) \\ &= e^{anh}T^n(\infty) + \frac{e^{anh}}{2\pi\imath}\int_{\Gamma+ah}\left[T^n(z) - T^n(\infty) - v(z)e^{-nz}y^T(z)\right](zI - hA)^{-1}dz. \end{aligned} \tag{35}$$

Here $\Gamma + ah$ is the positively oriented curve, lying in the resolvent set of the operator hA, equal to the union of the three portions

$$\Gamma_1 + ah = ah + \frac{e^{i\phi}}{n}, \quad \theta \leq \phi \leq 2\pi - \theta,$$

$$\Gamma_2 + ah = ah + re^{\pm i\theta}, \quad 1/n \leq r \leq R,$$

$$\Gamma_3 + ah = ah + re^{\pm i\theta}, \quad R \leq r \leq \infty.$$

Geometric considerations show that $\Gamma+ah \subset (\overline{B}(0,(\text{cosec}\,\theta)/n)\cup\overline{S}_{0,\theta})$ for all $ah \geq 0$ Hence we apply Lemma 7 to bound $\|T^n(z)-v(z)e^{-nz}y^T(z)\|$ in $(\Gamma_1+ah)\cup(\Gamma_2+ah)$. We will show that the right-hand side of (35) may be bounded by $C(ah+1/n)^p$, for some constant C independent of n,a, and h and hence deduce the theorem for $n \geq 2/R$. We will use inequality (3) and Lemma 7 tacitly.
Note that

$$\|e^{anh}T^n(\infty)\| \leq e^{anh}C\Lambda^n \leq C\Lambda^{n/2}.$$

Hence, for n sufficiently large it is possible to find another positive constant (independent of n,a,and h) denoted again by C, such that

$$\|e^{anh}T^n(\infty)\| \leq C(1/n+ah)^p.$$

Hence, taking the norm of the two sides of (35), we deduce

$$e^{anh}\|(T^n(hA)-v(hA)e^{-nhA}y^T(hA)\|$$

$$\leq \|e^{anh}T^n(\infty)\| + \|\frac{e^{anh}}{2\pi i}\int_{\Gamma+ah}\left[T^n(z)-T^n(\infty)-v(z)e^{-nz}y^T(z)\right](zI-hA)^{-1}dz\|. \tag{36}$$

Using the form of $\Gamma+ah$

$$\|\frac{e^{anh}}{2\pi i}\int_{\Gamma+ah}\left[T^n(z)-T^n(\infty)-v(z)e^{-nz}y^T(z)\right](zI-hA)^{-1}dz\| \leq \|I_1\|+\|I_2\|+\|I_3\|,$$

where

$$I_k = \frac{e^{anh}}{2\pi i}\int_{\Gamma_k+ah}\left[T^n(z)-T^n(\infty)-v(z)e^{-nz}y^T(z)\right](zI-hA)^{-1}dz, \qquad k=1,2,3,$$

and Γ_k, $k=1,2,3$ are the contours described above. Hence,

$$
\begin{aligned}
\|I_1\| \;&\le \frac{M}{2\pi}\int_{\Gamma_1+ah}\frac{C\Lambda^{n/2}+\|e^{anh}(T^n(z)-v(z)e^{-nz}y^T(z))\|}{|z-ah|}|dz| \\
&\le \frac{M}{2\pi}\int_{\Gamma_1+ah}\frac{C\Lambda^{n/2}+e^{anh}C(\Lambda^n+|z^pe^{-nz}|)}{|z-ah|}|dz| \\
&\le \frac{M}{2\pi}\int_{\Gamma_1+ah}\frac{C\Lambda^{n/2}+C|z^pe^{-n(z-ah)}|}{|z-ah|}|dz| \\
&\le \frac{M}{2\pi}\int_{\Gamma_1}\frac{C\Lambda^{n/2}+C(|y|+ah)^p|e^{-ny}|}{|y|}|dy| \\
&\le \frac{M}{2\pi}\int_{\theta}^{2\pi-\theta} C\Lambda^{n/2}+C(1/n+ah)^p d\theta \\
&\le MC(\Lambda^{n/2}+(1/n+ah)^p)\le C(1/n+ah)^p.
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
\|I_2\| \;&\le \frac{M}{2\pi}\int_{\Gamma_2+ah}\frac{C\Lambda^{n/2}+C(\Lambda^n+|z^pe^{-n(z-ah)}|)}{|z-ah|}|dz| \\
&\le \frac{M}{2\pi}\int_{\Gamma_2}\frac{C\Lambda^{n/2}+C(|y|+ah)^p|e^{-ny}|}{|y|}|dy| \\
&\le \frac{M}{2\pi}\int_{1/n}^{R}\frac{C\Lambda^{n/2}+C(r+ah)^pe^{-nrcos\theta}}{r}dr \\
&\le \frac{MC\Lambda^{n/2}}{2\pi}\log(nR)+\frac{MC}{2\pi}\int_{1/n}^{R}\frac{(r+ah)^pe^{-nrcos\theta}}{r}dr. \qquad (37)
\end{aligned}
$$

Consider the first term in the right-side of (37). Note that there exists $n_0 \in \mathbb{N}$ and another constant denoted again by C, such that for all $n \ge n_0$

$$
\frac{MC\Lambda^{n/2}}{2\pi}\log(nR)\le C(1/n+ah)^p. \qquad (38)
$$

Consider now the second term in the right-side of (37), using changes of variables

$$
\begin{aligned}
&\int_{1/n}^{R} \frac{(r+ah)^p e^{-nr\cos\theta}}{r} dr \sum_{j=0}^{p} \left(\begin{array}{c} p \\ j \end{array}\right) (ah)^{p-j} \int_{1/n}^{R} r^{j-1} e^{-nr\cos\theta} dr \\
&= (ah)^p \int_{1/n}^{R} \frac{e^{-nr\cos\theta}}{r} dr + \sum_{j=1}^{p} \left(\begin{array}{c} p \\ j \end{array}\right) (ah)^{p-j} \int_{1/n}^{R} r^{j-1} e^{-nr\cos\theta} dr \\
&\leq (ah)^p \int_{\frac{\cos\theta}{2}}^{\infty} \frac{e^{-\gamma}}{\gamma} d\gamma + \sum_{j=1}^{p} \left(\begin{array}{c} p \\ j \end{array}\right) (ah)^{p-j} \int_{0}^{\infty} (2\sec\theta)^j \gamma^{j-1} e^{-\gamma} d\gamma \\
&\leq C_1 (ah)^p + C_2 \sum_{j=1}^{p} \left(\begin{array}{c} p \\ j \end{array}\right) (ak)^{p-j} (\frac{1}{n})^j \leq C(1/n+ah)^p.
\end{aligned} \tag{39}
$$

Hence, using (38) and (39) $\|I_2\| \leq C(1/n+ah)^p$. Finally, consider I_3

$$
\begin{aligned}
\|I_3\| \ &\leq \frac{M}{2\pi} \int_{\Gamma_3+ah} \frac{e^{anh}\|T^n(z)-T^n(\infty)\| + C|e^{-n(z-ah)}|}{|z-ah|} |dz| \\
&\leq \frac{M}{2\pi} \int_{\Gamma_3+ah} \frac{e^{anh}\Lambda^n}{|z||z-ah|} + \frac{C|e^{-n(z-ah)}|}{|z-ah|} |dz| \\
&\leq \frac{CM}{2\pi} \int_{\Gamma_3} \frac{\Lambda^{n/2}}{|y+ah||y|} + \frac{|e^{-ny}|}{|y|} |dy| \\
&\leq \frac{CM}{2\pi} \int_{R}^{\infty} \frac{1}{r} \left(\frac{\Lambda^{n/2}}{r} + e^{-nr\cos\theta} \right) dr
\end{aligned}
$$

Note that the function $re^{-rn\cos\theta}$ for $r \in [R,\infty[$,

$$
re^{-rn\cos\theta} = re^{-\frac{rn\cos\theta}{2}} e^{-\frac{rn\cos\theta}{2}} \leq re^{-\frac{rn\cos\theta}{2}} \Lambda^{n/2}.
$$

Let $C = \max_{r\in[R,\infty)} re^{-\frac{rn\cos\theta}{2}} < \infty$, we obtain $e^{-rn\cos\theta} \leq C\dfrac{\Lambda^{n/2}}{r}$ and therefore

$$
\|I_3\| \ \leq \frac{CM}{2\pi} \int_{R}^{\infty} \frac{1}{r} \left(\frac{\Lambda^{n/2}}{r} + e^{-nr\cos\theta} \right) dr \leq \frac{CM}{2\pi} \int_{R}^{\infty} \frac{\Lambda^{n/2}}{r^2} dr \leq C(1/n+ah)^p.
$$

Consider the case $n \in [1, 2/R]$. We may similarly bound the right-hand side of (36). Now the curve $\Gamma + ah$ equals to the union of the two portions $\Gamma = \Gamma_3 \cup \Gamma_4$, where

$$
\Gamma_4 = Re^{i\phi}, \qquad \theta \leq \phi \leq 2\pi - \theta.
$$

Consider

$$\|\frac{e^{anh}}{2\pi i}\int_{\Gamma_4+ah}\left(T^n(\infty)+(T^n(z)-v(z)e^{-nz}y^T(z))\right)(zI-hA^{-1})dz\|$$

$$\leq \frac{M}{2\pi}\int_{\Gamma_4+ah}\frac{C\Lambda^{n/2}+C(\Lambda^n+|z^p e^{-n(z-ah)}|)}{|z-ah|}|dz|$$

$$\leq \frac{M}{2\pi}\int_{\Gamma_4}\frac{C\Lambda^{n/2}+C(|y|+ah)^p e^{-nR\cos\theta}}{|y|}|dy|$$

$$\leq CM(1/n+ah)^p+CM(R+ah)^p\leq C(1/n+ah)^p.$$

Hence, we may choose C_0 so that (33) holds for all $n\in\mathbb{N}$. Since e^{-nhA} is a bounded linear operator, so is $T^n(hA)$ and hence the latter is well defined. □

The technique adopted to prove Theorem 10 has been introduce by Kreiss [20] and used by Lubich [24] (see also [13]) and Hill and Süli [17]. Although our proof is similar to that used in [17], our approach to bound (35) is different.

4.1 Examples and conclusions

We present now a class of multistep methods verifying the technical hypothesis on $\lambda_1(z)$. Consider the (ρ,σ) method defined by

$$\begin{aligned}\rho(w)&=\tfrac{1}{2}[(w^2-1)+\gamma(w-1)^2],\\ \sigma(w)&=\tfrac{1}{4}[(w+1)^2+\delta(w^2-1)+\varepsilon(w-1)^2],\end{aligned}\tag{40}$$

for $\gamma,\delta,\varepsilon\in\mathbb{R}$ (see [5]). The polynomial $P(w;z)$ is

$$P(w;z)=\frac{1}{4}a(z)w^2+\frac{1}{2}b(z)w+\frac{1}{4}c(z),\tag{41}$$

where

$$\begin{aligned}a(z)&=(\delta+\varepsilon+1)z+2(\gamma+1),\\ b(z)&=(1-\varepsilon)z-2\gamma,\\ c(z)&=(\varepsilon-\delta+1)z+2(\gamma-1).\end{aligned}$$

A double w root for (41) occurs when $b(z)^2-a(z)c(z)=0$. By simple calculations, we find that double roots must occur in the left half of the complex plane and hence, taking into account Lemma 1, outside the region $S_{0,\theta}\cup N_0$, for any $\theta\in(0,\pi/2)$, if

$$4\varepsilon<\delta^2,\qquad \delta>2\gamma.\tag{42}$$

Moreover, the method (40) is irreducible and A-stable for any $\gamma,\delta,\varepsilon$ such that

$$0\leq\gamma,\delta-\gamma,\varepsilon,\qquad 0<\max\{\varepsilon,\gamma(\delta-\gamma)\}.\tag{43}$$

Choosing for instance $\gamma = 0, \varepsilon = 1, \delta = 3$, we obtain the (ρ, σ) method defined by

$$\rho(w) = \frac{1}{2}(w^2 - 1), \qquad \sigma(w) = \frac{1}{4}(5w^2 - 1).$$

The two eigenvalues of the companion matrix $T(z)$ are $\lambda(z) = \pm\sqrt{\frac{2+z}{2+5z}}$ and they coincide at $z_0 = -2 \in \mathbb{C}^-$.

Note that the further condition $\delta = \gamma$ implies that the method (40) is second order, therefore conditions (42) and (43) hold for a range of first order, 2-step methods. In particular, consider the second-order BDF method (for $\delta = \gamma = 2$ and $\varepsilon = 1$)

$$\frac{3}{2}U^{n+2} - 2U^{n+1} + \frac{1}{2}U^n = hF^{n+2},$$

the two eigenvalues of $T(z)$ are $\lambda(z) = \dfrac{2 \pm \sqrt{1-2z}}{3+2z}$, and they coincide at the point $z_0 = \frac{1}{2} \in \mathbb{C}^+$.

To finish up we summerise our results. Consider first Theorem 10. This provides an optimal error bound for the approximation of e^{-At} by $T^n(hA)$ with a technical hypothesis on $\lambda_1(z)$, the principal eigenvalue of the companion matrix of the method. Our hypothesis consists that $\lambda_1(z)$ is simple for all points in a sector contained in the right-half of the complex plane. This does not prove to be too restrictive however, as we have seen, all the given examples of multistep methods which satisfy this condition have a first order accuracy. Therefore, it is clear that it is necessary to extend our error bound for the case of multiple roots because the companion matrix of some well-known, high order, multistep methods may possess multiple eigenvalues at some z belonging to $\mathbb{C}^+$. The real problem in this case appears to be the evaluation of the Dunford-Taylor integral along a cut integration contour and at present it is not clear how to solve this question. However, the linear theory in this paper and its optimal error bound represent the starting point for high-order study of the nonlinear case and of existence and convergence both of attractors and inertial manifolds.

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