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Rational inversion of the Laplace transform

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Abstract. This paper studies new inversion methods for the Laplace transform of vector-valued functions arising from a combination of A-stable rational approximation schemes to the exponential and the shift operator semigroup. Each inversion method is provided in the form of a (finite) linear combination of the Laplace transform of the function and a finite amount of its derivatives. Seven explicit methods arising from A-stable schemes are provided, such as the Backward Euler, RadauIIA, Crank-Nicolson, and Calahan scheme. The main result shows that, if a function has an analytic extension to a sector containing the nonnegative real line, then the error estimate for each method is uniform in time.

Introduction

The numerical inversion of the Laplace transform has been studied by many authors over the years due to the wide array of applications of the Laplace transform technique to different areas of science. If $u : [0, \infty) \to X$, where X is a Banach space and assuming that its Laplace transform $\widehat{u}(\lambda) := \int_0^\infty e^{-\lambda t} u(t)\,\mathrm{d}t$ exists for some $\lambda \in \mathbb{C}$, then it can be shown that there exist an $\omega \in \mathbb{R}$ such that $\widehat{u}$ is analytic on $H_\omega := \{\lambda \in \mathbb{C} : \mathrm{Re}(\lambda) > \omega\}$, see [1, Sec 1.4]. The problem is to find an operator $L_n[\widehat{u}, t]$ such that $\lim_{n\to\infty} L_n[\widehat{u}, t] = u(t)$ for each $t \geq 0$ and, more importantly, to estimate the error $\|L_n[\widehat{u}, t] - u(t)\|$ in the Banach space norm.

The inversion problem for the Laplace transform has been cataloged by some authors as more of an art than a science because most methods use several parameters that need to be adjusted in order to obtain reasonable results or because most methods work only for very particular functions, cf. [8]. One of the most successful methods for inverting the Laplace transform is Talbot's method, also known as the quadrature method (see [29,44,48,49]). Before the methods presented in this paper, the quadrature method and the Post-Widder method were the only available methods for inverting the Laplace transform of Banach-space-valued functions. The quadrature method assumes that the Laplace transform $\widehat{u}$ has an analytic extension beyond H_ω. However, it is not hard to find functions whose Laplace transform does not have an analytic extension beyond H_ω. On the other hand, the Post-Widder inversion method defines an operator L_n using

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the first $n-1$ derivatives of $\widehat{u}$ with order of convergence $\frac{t}{\sqrt{n}}$, making the Post-Widder inversion method to be extremely slow as $n \to \infty$.

This paper studies error estimates for a new class of rational Laplace transform inversion procedures by defining an operator L_n which uses the information of $\widehat{u}(\lambda)$ and the first $n-1$ derivatives of $\widehat{u}$ on H_ω for any continuous and exponentially bounded function u with values in a Banach space X with an order of convergence $\frac{t}{n^m}$ for some $m \in \mathbb{N}$. In fact, for each $m \in \mathbb{N}$ we can find an approximation method for the inverse Laplace transform with order of convergence $\frac{t}{n^m}$. Therefore, one can keep the order of derivatives of $\widehat{u}$ low by considering m big enough and, at the same time, there is no requirement for an analytic extension of $\widehat{u}$ beyond its natural domain H_ω. The main contribution of the present paper is the characterization of those functions for which the inversion methods provide time-independent error estimates, i.e., with rate of convergence $\frac{1}{n^m}$ for any $t \in [0, \infty)$. The rational Laplace transform inversion methods are derived from the theory of rational approximation methods for operator semigroups using results due to Hersh and Kato [16], Brenner and Thomée [5], Larsson, Thomée, and Wahlbin [30], Hansbo [15], and Crouzeix, Larsson, Piskarev, and Thomée [7] (see also [24,25] and [45]). They first appear as an example of rational approximations to bi-continuous semigroups in [19].

The first section of this work compiles the results concerning rational approximations of operator semigroups emphasizing the approximation results for the shift semigroup $e^{t\partial}$ on Banach spaces $\mathbb{X}$ of continuous functions u with the sup-norm. Section 1 contains the main results concerning the error analysis for the inversion of the Laplace transform via $\mathcal{A}$-stable rational approximations to the exponential. Sections 2, 3, and 4 implement different rational inversion schemes associated to Subdiagonal Padé approximants, Restricted Padé approximants, and Composite Exponential approximations, respectively. The last section provides a comparison of the rational inversion Laplace transform method with the quadrature method as well as some applications to differential equations with numerical examples.

1. Rational approximation of operator semigroups

In this section we compile the results concerning rational approximation of operator semigroups needed for the rational Laplace transform inversion method.

Let $r = \frac{P}{Q}$ be an $\mathcal{A}$-stable rational approximation to the exponential function of order m, i.e., P and Q are polynomials with $p := deg(P) \leq deg(Q) =: q$, and

(i) $|r(z) - e^z| \leq C_m |z|^{m+1}$ for $|z|$ sufficiently small, and
(ii) $|r(z)| \leq 1$ for $\mathrm{Re}(z) \leq 0$.

It is a well-known result of Padé [34] that $m \leq p+q$ for all rational approximations to the exponential function. The rational approximations of maximal order $m = p+q$ are called *Padé* approximations. They are of the form $r_{\{p,q\}} = \frac{P}{Q}$, where

$$P(z) = \sum_{j=0}^{p} \frac{(m-j)!p!}{m!j!(p-j)!} z^j \quad \text{and} \quad Q(z) = \sum_{j=0}^{q} \frac{(m-j)!q!}{m!j!(q-j)!} (-z)^j. \tag{1}$$

As shown in [10], Padé approximations are $\mathcal{A}$-stable if and only if $q-2 \le p \le q$. Another class of rational approximations to the exponential function are the *restricted Padé* approximants

$$r_{\{n\}}(z) = \frac{\sum_{j=0}^{n} (-1)^n L_n^{(n-j)}(1/b)(bz)^j}{(1-bz)^n}, \tag{2}$$

where L_n denotes the nth Laguerre polynomial $L_n(x) = \sum_{j=0}^{n} (-1)^j \binom{n}{j} \frac{x^j}{j!}$. They are of order $m = n+1$ for suitable $b \in \mathbb{R}$. It was shown by G. Wanner, E. Hairer, and S. P. Nørsett [47] (see also [14]) that the only $\mathcal{A}$-stable restricted Padé approximants of order $m = n+1$ are $r_{\{1\}}$, $r_{\{2\}}$, $r_{\{3\}}$, and $r_{\{5\}}$.

LEMMA 1. *If r is an $\mathcal{A}$-stable rational approximation to the exponential of order $m \ge 1$, then $|r^n(\frac{t}{n}z) - e^{tz}| \le C_m t^{m+1} \frac{1}{n^m} |z^{m+1}|$ for $Re(z) \le 0$ and $t \ge 0$.*

Proof. By the binomial formula, $|r^n(\frac{t}{n}z) - e^{tz}| = |r^n(\frac{t}{n}z) - (e^{\frac{t}{n}z})^n| = \left|\sum_{j=0}^{n-1} r(\frac{t}{n}z)^{n-1-j} (e^{\frac{t}{n}z})^j\right| \cdot |r(\frac{t}{n}z) - e^{\frac{t}{n}z}| \le nC_m |\frac{tz}{n}|^{m+1} = C_m t^{m+1} \frac{1}{n^m} |z|^{m+1}$. □

The papers [5,7,16], and [30] contain some of the main results for rational approximation schemes $V(t) := r(tA)$ for strongly continuous operator semigroups $T(t) = e^{tA}$ generated by a linear operator A with domain $D(A)$ and range in a Banach space $\mathbb{X}$, where r is an $\mathcal{A}$-stable rational approximation to the exponential function of order m.

It is one of the key results in the approximation theory for operator semigroups (Theorem 2 below) that Lemma 1 holds if z is replaced by the generator A of a bounded strongly continuous semigroup $T(t) = e^{tA}$ on a Banach space $\mathbb{X}$; i.e.,

$$\left\| r^n\left(\frac{t}{n}A\right)u - e^{tA}u \right\|_{\mathbb{X}} \le \tilde{C}_m t^{m+1} \frac{1}{n^m} \|A^{m+1}u\|_{\mathbb{X}} \tag{3}$$

for all $u \in D(A^{m+1})$. Moreover, if r is an $\mathcal{A}$-stable approximation to the exponential, then $r^n(\frac{t}{n}A)u - e^{tA}u \to 0$ for all $u \in \mathbb{X}$ if and only if the operators $V(t) := r(tA)$ are stable; i.e., there exist $\omega, M \ge 0$ such that $\|V^n(\frac{t}{n})\| \le Me^{\omega t}$ for each $n \in \mathbb{N}_0$ and $t \ge 0$. This follows from the celebrated result of Lax and Richtmyer [28] and, in final form, given by Chernoff in [6] (see also [11]) which asserts that if $\{V(t); t \ge 0\} \subset \mathcal{L}(\mathbb{X})$ is an approximation scheme with $V(0) = I$ and $V'(0^+)u = Au$ for all u in a dense set $D \subset D(A)$, then (i) $V(t)$ is stable if and only if (ii) $\lim_{n\to\infty} V^n(\frac{t}{n})u = T(t)u$ for all $t \ge 0$ and $u \in \mathbb{X}$.

Approximation schemes $V(t) = r(tA)$ defined by $\mathcal{A}$-stable rational approximation r to the exponential of order $m \ge 1$ were investigated in the ground-breaking papers of Hersh and Kato [16] and Brenner and Thomée [5]. The following theorem summarizes the results obtained in [5].

THEOREM 2. *Let A be the generator of a strongly continuous semigroup $T(t)$ with $\|T(t)\| \leq Me^{\omega t}$ for some $M, \omega > 0$. If $V(t) := r(tA)$ for some $\mathcal{A}$-stable rational approximation r to the exponential or order $m \geq 1$, then $V(\cdot)$ may not be stable. However, there are constants C_m, κ such that for all $t \geq 0$*

$$\left\| r^n\left(\frac{t}{n}A\right)\right\|_{\mathcal{L}(\mathbb{X})} \leq C_m M\sqrt{n}e^{\omega\kappa t}.$$

If $k = 0, 1, \ldots, m+1$ with $k \neq \frac{m+1}{2}$, then there are $C_m > 0$ (depending only on r) such that

$$\left\| r^n\left(\frac{t}{n}A\right)u - T(t)u\right\|_{\mathbb{X}} \leq C_m M e^{c\omega t} t^k \left(\frac{1}{n}\right)^{\beta(k)} \|A^k u\|_{\mathbb{X}}$$

for every $t \geq 0, n \in \mathbb{N}$, and $u \in D(A^k)$, where

$$\beta(k) := \begin{cases} k - \frac{1}{2} & \text{if } 0 \leq k < \frac{m+1}{2}, \\ k\frac{m}{m+1} & \text{if } \frac{m+1}{2} < k \leq m+1. \end{cases}$$

If $k = \frac{m+1}{2}$, then for every $t \geq 0, n \in \mathbb{N}$, and $u \in D(A^{\frac{m+1}{2}})$,

$$\left\| r^n\left(\frac{t}{n}A\right)u - T(t)u\right\|_{\mathbb{X}} \leq C_m M e^{\omega t} t^{\frac{m+1}{2}} \left(\frac{1}{n}\right)^{m/2} \ln(n+1)\|A^{\frac{m+1}{2}}u\|_{\mathbb{X}}.$$

REMARK 3. (i) The theorem above extends to generators of bi-continuous semigroups and C-regularized semigroups, see [18–20]. In particular, Theorem 2 applies to the shift semigroup on the space $\mathbb{X}$ of bounded and continuous functions with values in a Banach space X denoted by $\mathcal{C}_b(\mathbb{R}^+, X)$ with sup-norm, in which case the generator $\partial := \frac{d}{ds}$ is not densely defined.

(ii) The error estimates given in Theorem 2 extend to initial values in a continuum of intermediate spaces between the Banach space $\mathbb{X}$ and the domain of the nth powers of generators of strongly continuous semigroups, see [25].

(iii) The estimates are sharp for the shift semigroup on $\mathbb{X} = \mathcal{C}_b(\mathbb{R}^+, X)$ given by $T(t)u : s \to u(s+t)$ with $r(z) = \frac{2+z}{2-z}$ (Crank-Nicolson), see [19].

(iv) It is shown in [5] that if an $\mathcal{A}$-stable rational approximation r satisfies
  (a) $|r(is)| < 1$ for $s \in \mathbb{R} - \{0\}$ and $|r(\infty)| < 1$,
  (b) $r(is) = e^{is+\psi(s)}$ with $\psi(s) = O(|s|^{\tilde{q}+1})$ for positive integer $\tilde{q}$ as $s \to 0$,
  (c) $\mathrm{Re}\psi(s) \leq -\gamma s^{\tilde{p}}$ for $|s| \leq 1$ and some even integer $\tilde{p} \geq \tilde{q}+1$,

  then $\|r^n(\frac{t}{n}A)\|_{\mathcal{L}(\mathbb{X})} \leq C_m M n^{(\frac{1}{2}-\frac{\tilde{q}+1}{2\tilde{p}})} e^{\omega\kappa t}$ and Theorem 2 holds with $\beta(k)$ replaced by

$$\beta_*(k) := k\frac{\tilde{q}}{\tilde{q}+1} + \min\left\{0, \left(k - \frac{1}{2}(\tilde{q}+1)\right)\left(\frac{1}{\tilde{q}+1} - \frac{1}{\tilde{p}}\right)\right\}.$$

(v) The first subdiagonal Padé approximants $r_{\{j-1,j\}}$ are of order $m = 2j-1$ and (iv) holds with $\tilde{p} = 2j$ and $\tilde{q} = 2j-1$, see [5]. In particular,

$$\left\| r^n\left(\frac{t}{n}A\right)\right\|_{\mathcal{L}(\mathbb{X})} \leq C_m M e^{\omega\kappa t}$$

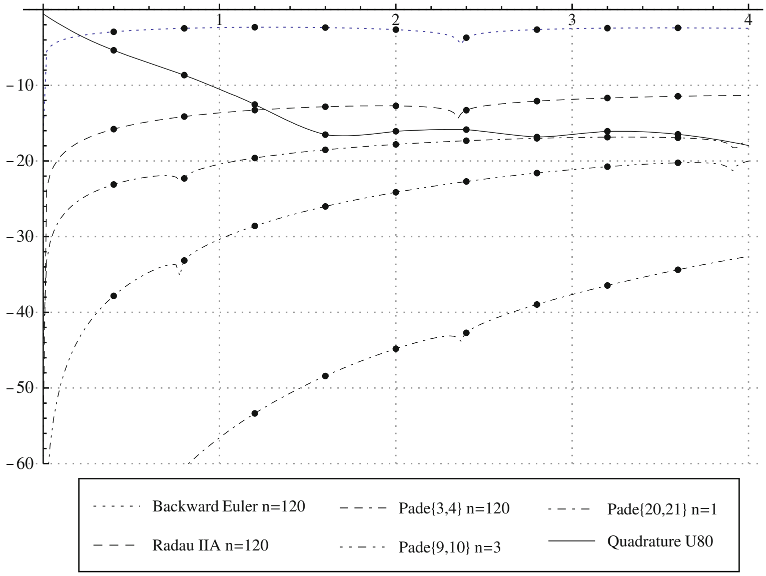

Figure 1. Logarithmic error $\log_{10}(E(n, t, u))$ for different schemes provided by Padé approximants and the quadrature method $U80$ (see Table 1 of [39]) for the approximation of the solution u of (16) for $t \in [0, 4]$

for all $t \geq 0$ and $\beta_*(k) = k\frac{m}{m+1}$ for $0 \leq k \leq m+1$, $k \neq j$; i.e., the subdiagonal Padé schemes are stable.

(vi) The restricted Padé approximant $r_{\{2\}}$ (Calahan) has order $m = 3$ and (iv) holds with $\tilde{p} = 4$ and $\tilde{q} = 3$. Thus, $r^n_{\{2\}}(\frac{t}{n}A)$ is stable and $\beta_*(k) = \frac{3k}{4}$, [5].

(vii) The restricted Padé approximant $r_{\{3\}}$ has order $m = 4$ and (iv) holds with $\tilde{p} = 6$ and $\tilde{q} = 4$. In particular, $r^n_{\{3\}}(\frac{t}{n}A)$ is $O(\sqrt[12]{n})$ and $\beta_*(1) = \frac{3}{4}$, see [5].

(viii) For $\mathcal{A}$-stable rational approximation schemes for which $r(tA)$ is stable, the factor $\ln(n+1)$ can be removed. See [12] and Corollary 4.4 in [25].

(ix) A precise estimate for the constant $C_m = C(r_m)$ for an $\mathcal{A}$-stable approximation r_m to the exponential of order m is an open problem. A preliminary result can be found in Lemma III.8 of [40]. Moreover, numerical evidence suggests that $C_m \to 0$ as $m \to \infty$, see Fig. 1 for $n = 1$.

Time-independent convergence estimates for $\mathcal{A}$-stable rational approximations can be obtained for bounded *analytic* semigroups as attained by Larsson, Thomée, and Wahlbin [30] and Crouzeix, Larsson, Piskarev, and Thomée [7] (see also [45]). Their results are summarized in the following theorem.

THEOREM 4. *Let A be the generator of an analytic semigroup $T(t)$ on $\mathbb{X}$ with $\|T(t)\|_{\mathcal{L}(\mathbb{X})} \leq M$ ($t \geq 0$). If r is an $\mathcal{A}$-stable rational approximation to the exponential of order $m \geq 1$, then there is a constant C_m satisfying*

(a) $\|r^n(\frac{t}{n}A)\|_{\mathcal{L}(\mathbb{X})} \leq C_m M$ *for* $t \geq 0$, *and*
(b) $\|r^n(\frac{t}{n}A)u - T(t)u\|_{\mathbb{X}} \leq C_m M \left(\frac{t}{n}\right)^m \|A^m u\|_{\mathbb{X}}$ *for* $t \geq 0,\ u \in D(A^m)$.
(c) *If* $|r(\infty)| < 1$ *then* $\|r^n(\frac{t}{n}A)u - T(t)u\|_{\mathbb{X}} \leq C_m M \frac{1}{n^m}\|u\|_{\mathbb{X}}$ *for* $t \geq 0,\ u \in \mathbb{X}$.

Even though $\mathcal{A}$-stable rational approximations r are stable for analytic semigroups $T(t)$ generated by A, the convergence $r^n(\frac{t}{n}A)u \to T(t)u$ can be arbitrarily slow for non-smooth initial data $u \in \mathbb{X}$ if $|r(\infty)| = 1$ (e.g., Crank-Nicolson). The stabilization of rational approximation schemes for non-analytic strongly continuous semigroups was investigated by McAllister and Neubrander in [31].

Let X be a Banach space. We denote by $\mathcal{C}_b(\mathbb{R}^+, X)$ the Banach space of bounded and continuous functions from $\mathbb{R}^+$ into X and $\mathcal{C}_0(\mathbb{R}^+, X) := \{u \in \mathcal{C}_b(\mathbb{R}^+, X) : u(\infty) = 0\}$. Let Σ_θ be the sector $\{z \in \mathbb{C}\backslash\{0\} : |arg(z)| < \theta\}$, $H(\Sigma_\theta, X)$ the space of all analytic functions $u : \Sigma_\theta \to X$, and $C_{ub}(\overline{\Sigma_\theta}, X)$ the space of all bounded, uniformly continuous functions from Σ_θ into X. For a proof of the following statements, see [2] and [19].

PROPOSITION 5. *The shift semigroup* $T(t)u : s \to u(s+t)$ *is bi-continuous on* $\mathbb{X} = \mathcal{C}_b(\mathbb{R}^+, X)$, *strongly continuous on* $\mathbb{X} = \mathcal{C}_0(\mathbb{R}^+, X)$, *and bounded and analytic on* $\mathbb{X} = C_{ub}(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$.

2. Rational Laplace transform inversion

This section shows that approximation methods for semigroups of operators yield sharp inversion methods for the Laplace transform. This follows by applying the results of Theorem 2 and Remark 3 to the shift semigroup $T(t)u : s \to u(t+s)$ with generator $A = \partial := d/ds$ on the spaces of continuous functions described in Proposition 5. The operator ∂ is always considered on its maximal domain; i.e., $D(\partial) = \{u \in \mathbb{X} : u' \in \mathbb{X}\}$.

Let X be a Banach space. Consider the shift semigroup $T(t)u : s \to u(t+s)$ on $\mathbb{X} = \mathcal{C}_0(\mathbb{R}^+, X)$ (or $\mathcal{C}_b(\mathbb{R}^+, X)$ or $C_{ub}(\overline{\Sigma_\theta}, X)$). Then, by Proposition 5, $T(t)$ is a strongly continuous (bi-continuous, analytic) semigroup with generator $\partial = d/ds$, where $D(\partial) = \{u \in \mathbb{X} : u' \in \mathbb{X}\}$ and the resolvent operator is denoted by $R(\lambda, \partial) := (\lambda - \partial)^{-1}$. Since

$$R(\lambda, \partial)u = \int_0^\infty e^{-\lambda t} T(t)u \,\mathrm{d}t = \int_0^\infty e^{-\lambda t} u(t + \cdot) \,\mathrm{d}t,$$

it follows that

$$R(\lambda, \partial)u(0) = \int_0^\infty e^{-\lambda t} u(t) \,\mathrm{d}t = \widehat{u}(\lambda)$$

(the Laplace transform of u). Consequently,

$$\begin{aligned} R(\lambda, \partial)^{n+1}u(0) &= \frac{(-1)^n}{n!} R(\lambda, \partial)^{(n)} u(0) \\ &= \frac{(-1)^n}{n!} \int_0^\infty e^{-\lambda t} (-t)^n u(t) \,\mathrm{d}t = \frac{(-1)^n}{n!} \widehat{u}^{(n)}(\lambda). \end{aligned}$$

Now, let $r(z) = \frac{P(z)}{Q(z)}$ be an $\mathcal{A}$-stable rational approximation to the exponential function of order $m \geq 1$. Then, using partial fraction decomposition, there exist constants $B_0, B_{\{1,i,j\}}, b_i \in \mathbb{C}$ with $Re(b_i) > 0$, and $r_i \in \mathbb{N}$ such that

$$r(z) = B_0 + \sum_{i=1}^{s} \sum_{j=1}^{r_i} \frac{B_{\{1,i,j\}}}{(b_i - z)^j}.$$

Thus, for each $n \in \mathbb{N}$, there exist constants $B_{\{n,i,j\}} \in \mathbb{C}$ such that

$$r^n(z) = B_0^n + \sum_{i=1}^{s} \sum_{j=1}^{nr_i} \frac{B_{\{n,i,j\}}}{(b_i - z)^j}. \tag{4}$$

In particular,

$$\begin{aligned} r^n\left(\frac{t}{n}\partial\right)u(0) &= B_0^n u(0) + \sum_{i=1}^{s}\sum_{j=1}^{nr_i} B_{\{n,i,j\}} R\left(b_i, \frac{t}{n}\partial\right)^j u(0) \\ &= B_0^n u(0) + \sum_{i=1}^{s}\sum_{j=1}^{nr_i} B_{\{n,i,j\}} \left(\frac{n}{t}\right)^j R\left(\frac{nb_i}{t}, \partial\right)^j u(0) \\ &= B_0^n u_0 + \sum_{i=1}^{s}\sum_{j=1}^{nr_i} B_{\{n,i,j\}} \left(\frac{n}{t}\right)^j \frac{(-1)^{j-1}}{(j-1)!}\widehat{u}^{(j-1)}\left(\frac{nb_i}{t}\right), \end{aligned}$$

where $u_0 := \lim_{\lambda\to\infty} \lambda\widehat{u}(\lambda) = u(0)$. Since $T(t)u(0) = u(t)$, it follows that the approximation error

$$\begin{aligned} E_m(n,t,u) &:= \left\| B_0^n u_0 + \sum_{i=1}^{s}\sum_{j=1}^{nr_i} B_{\{n,i,j\}} \left(\frac{n}{t}\right)^j \frac{(-1)^{j-1}}{(j-1)!}\widehat{u}^{(j-1)}\left(\frac{nb_i}{t}\right) - u(t)\right\| \\ &= \left\| r^n\left(\frac{t}{n}\partial\right)u(0) - u(t)\right\| = \left\| r^n\left(\frac{t}{n}\partial\right)u(0) - T(t)u(0)\right\| \end{aligned}$$

can be estimated by

$$\begin{aligned} E_m(n,t,u) &\leq \left\| r^n\left(\frac{t}{n}\partial\right)u - T(t)u\right\|_\infty := \sup_{s\in[0,\infty)} \left\| r^n\left(\frac{t}{n}\partial\right)u(s) - T(t)u(s)\right\| \\ &= \left\| r^n\left(\frac{t}{n}\partial\right)u - T(t)u\right\|_{\mathbb{X}}. \end{aligned} \tag{5}$$

Thus, the semigroup results of Theorems 2, Remark 3-(i), and Theorem 4 applied to the shift semigroup on the Banach spaces of continuous functions $\mathcal{C}_0(\mathbb{R}^+, X)$, or $\mathcal{C}_b(\mathbb{R}^+, X)$, or $C_{ub}(\overline{\Sigma_\theta}, X)$, respectively, yield the following result concerning the inversion of the Laplace transform.

THEOREM 6. (Rational Laplace Transform Inversion) *Let r be an $\mathcal{A}$-stable rational approximation to the exponential function of order $m \geq 1$ with constants*

$B_0, B_{\{1,i,j\}}, b_i \in \mathbb{C}, r_i \in \mathbb{N}$ as defined in (4). Let $u \in \mathbb{X} = \mathcal{C}_0(\mathbb{R}^+, X)$ (or $\mathcal{C}_b(\mathbb{R}^+, X)$ or $C_{ub}(\overline{\Sigma_\theta}, X)$), let $u_0 := \lim_{\lambda\to\infty} \lambda\widehat{u}(\lambda) = u(0)$, and consider

$$E_m(n, t, u) := \left\| B_0^n u_0 + \sum_{i=1}^{s} \sum_{j=1}^{nr_i} B_{\{n,i,j\}} \left(\frac{n}{t}\right)^j \frac{(-1)^{j-1}}{(j-1)!} \widehat{u}^{(j-1)} \left(\frac{nb_i}{t}\right) - u(t) \right\|.$$

Then, the following statements hold.

(i) *If $|r(\infty)| < 1$ and $u \in C_{ub}(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$, then for all $t \geq 0$,*

$$E_m(n, t, u) \leq C_m \frac{1}{n^m} \|u\|_\infty.$$

(ii) *If $|r(\infty)| = 1$ and $u, u^{(m+1)} \in C_{ub}(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$, then for all $t \geq 0$,*

$$E_m(n, t, u) \leq C_m t^m \frac{1}{n^m} \|u^{(m)}\|_\infty.$$

(iii) *If $u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X)$ for some $1 \leq k \leq m+1$, then for all $t \geq 0$,*

$$E_m(n, t, u) \leq C_m t^k \frac{1}{n^{\gamma(k)}} \|u^{(k)}\|_\infty,$$

where $\gamma(k)$ is given by $\beta(k)$ or $\beta_*(k)$ as defined in Theorem 2. In particular,

$$E_m(n, t, u) \leq \begin{cases} C_m t^{m+1} \frac{1}{n^m} \|u^{(m+1)}\|_\infty & \text{if } u, u^{(m+1)} \in \mathcal{C}_b(\mathbb{R}^+, X), \\ C_m t \frac{1}{n^\beta} \|u^{(1)}\|_\infty & \text{if } u, u^{(1)} \in \mathcal{C}_b(\mathbb{R}^+, X), \end{cases}$$

for all $t \geq 0$, where $\beta \in [\frac{1}{2}, 1)$ is given by $\beta(1)$ or $\beta_*(1)$ as defined in Theorem 2.

(iv) *If $V(t) := r(t\partial)$ is stable on one of the spaces $\mathbb{X}$ of continuous functions considered in Proposition 5, then for all $u \in \mathbb{X}$,*

$$\lim_{n\to\infty} E_m(n, t, u) = 0,$$

where the convergence is uniform on compact sets.

REMARK 7. In Theorem 6(iii), it seems to be unknown if there are rational schemes for which the order of convergence is $O(\frac{1}{n^\beta})$ for some $\beta \geq 1$ and all u with $u, u^{(1)} \in \mathcal{C}_b(\mathbb{R}^+, X)$.

Let $\mathcal{C}_{b,\omega}(\mathbb{R}^+, X)$ be the Banach space of continuous functions u from $\mathbb{R}^+$ into X for which $\|u\|_{\omega,\infty} := \sup_{t\geq 0} \|e^{-\omega t} u(t)\| < \infty$. Since the norm of the shift semigroup is bounded by $e^{\omega t}$ on $\mathcal{C}_{b,\omega}(\mathbb{R}^+, X)$, Theorem 2 yields also error estimates for rational Laplace transform inversions for $u \in \mathcal{C}_{b,\omega}(\mathbb{R}^+, X)$.

3. Subdiagonal Padé inversion of the Laplace transform

To provide a first example of rational Laplace transform inversion procedures, consider the subdiagonal Padé approximants $r_{\{s-1,s\}} := r$ with $r(z) = \frac{P(z)}{Q(z)}$, where P, Q

are as in (1)). These Padé approximants are $\mathcal{A}$-stable, of order $m = 2s - 1$, and the statements of Theorem 4 (c) and the Remark 3-(iv) of Theorem 2 hold. It is known (see, e.g., [14,41]) that r has s distinct poles b_i with $Re(b_i) > 0$. Thus, by using partial fraction decomposition,

$$r(z) = \sum_{i=1}^{s} \frac{B_{\{1,i,1\}}}{b_i - z}, \tag{6}$$

where $B_{\{1,i,1\}} = \frac{P(b_i)}{\prod_{k\neq i}(b_k - b_i)}$. If a rational function is of the form (3.1), then another partial fraction argument yields that, for each $n \in \mathbb{N}$,

$$r^n(z) = \sum_{i=1}^{s} \sum_{j=1}^{n} \frac{B_{\{n,i,j\}}}{(b_i - z)^j}, \tag{7}$$

where the constants $B_{\{n,i,k\}}$ $(1 \le i \le s,\ 1 \le k \le n)$ are inductively given by

$$\begin{aligned} B_{\{n+1,i,1\}} &= \sum_{k=1}^{n} \sum_{\substack{j=1\\ j\neq i}}^{s} a_{ij}^{k} \left[(-1)^{k+1} B_{\{n,i,k\}} \cdot B_{\{1,j,1\}} + B_{\{n,j,k\}} \cdot B_{\{1,i,1\}}\right] \\ B_{\{n+1,i,n+1\}} &= B_{\{n,i,n\}} \cdot B_{\{1,i,1\}} \\ B_{\{n+1,i,r\}} &= \left[\sum_{k=r}^{n} \sum_{\substack{j=1\\ j\neq i}}^{s} B_{\{n,i,k\}} \cdot B_{\{1,j,1\}} \cdot a_{ij}^{k-r+1} \cdot (-1)^{k-r}\right] \\ &\quad + B_{\{n,i,r-1\}} \cdot B_{\{1,i,1\}} \qquad \text{for all } 2 \le r \le n, \end{aligned} \tag{8}$$

and where $a_{ij} := \frac{1}{b_j - b_i}$. For the proof of (8) see [18, Lemma 3.2.4]. Thus, for a subdiagonal Padé approximation r to the exponential function of order $m = 2s - 1$ $(s \ge 1)$ with given poles $b_1, b_2, \ldots, b_s$, Theorem 6 is applicable with $B_0 = 0$ and $B_{\{n,i,j\}}$ given in (8). Observe that (i) and (iv) of Theorem 6 are applicable since $r(\infty) = 0$ and $r(tA)$ is stable for $A = d/ds$ on all spaces $\mathbb{X}$ of continuous functions considered above (see Remark 3-(v)). The numerical implementation of the subdiagonal rational Laplace transform inversion method rely on the accuracy of the roots of the polynomial Q for $s \ge 5$. For different methods concerning the numerical approximation of zeros of polynomials, we refer to [35,36], and the references therein. Symbolic tools of widely available software such as Maple, Mathematica, or Matlab provide fast algorithms to find the zeros of Q with arbitrary precision. However, in this case, it is important to use algorithms which calculate the roots of Q with high precision since the error growth of the recursion (7) is exponential as n increases. A simple Mathematica code for the scalar-valued case can be found in [18]. For $s = 1, 2, 3, 4, 11$ (respectively $m = 1, 3, 5, 7, 21$), the subdiagonal Padé inversions of the Laplace transform are as follows.

3.1. Backward Euler (Post-Widder) inversion ($m = 1$)

If $s = 1$ in (6), then $m = 2s - 1 = 1$ and the subdiagonal Padé approximation $r_{\{0,1\}}$ (Backward Euler) is given by

$$r(z) = \frac{1}{1-z}.$$

Since $r^n(z) = \frac{1}{(1-z)^n}$, (4) holds with $s = 1, r_1 = 1, b_1 = 1, B_0 = 0, B_{\{n,1,n\}} = 1$, and $B_{\{n,1,j\}} = 0$ for $j \neq n$. Thus, Theorem 6 holds for $m = 1$ and

$$E_1(n,t,u) := \left\| \frac{(-1)^{n-1}}{(n-1)!} \left(\frac{n}{t}\right)^n \widehat{u}^{(n-1)} \left(\frac{n}{t}\right) - u(t) \right\| \tag{9}$$

satisfies, for all $t \geq 0$,

$$E_1(n,t,u) \leq \begin{cases} C_1 t \frac{1}{\sqrt{n}} \|u^{(1)}\|_\infty & \text{if } u, u^{(1)} \in \mathcal{C}_b(\mathbb{R}^+, X) \\ C_1 t^2 \frac{1}{n} \|u^{(2)}\|_\infty & \text{if } u, u^{(2)} \in \mathcal{C}_b(\mathbb{R}^+, X), \\ C_1 \frac{1}{n} \|u\|_\infty & \text{if } u \in C_{ub}(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X). \end{cases}$$

Moreover, $\lim_{n\to\infty} E_1(n,t,u) = 0$ for all $u \in \mathcal{C}_b(\mathbb{R}^+, X)$ and the Backward Euler approximations (9) retain essential structural characteristics of u (positivity, monotonicity, convexity, etc.; see [17,26]). To see the connection between (9) and the Post-Widder inversion

$$\frac{(-1)^n}{n!} \left(\frac{n}{t}\right)^{n+1} \widehat{u}^{(n)} \left(\frac{n}{t}\right), \tag{10}$$

define $U(t) := \int_0^t u(r)\,dr$ and $\widehat{U}(\lambda) := \int_0^\infty e^{-\lambda t} U(t)\,\mathrm{d}t$. Since $\widehat{U}(\lambda) = \frac{1}{\lambda}\widehat{u}(\lambda)$ it follows that

$$\begin{aligned} \frac{(-1)^{n-1}}{(n-1)!} \left(\frac{n}{t}\right)^n \widehat{U}^{(n-1)} \left(\frac{n}{t}\right) &= \sum_{j=0}^{n-1} \frac{(-1)^j}{j!} \left(\frac{n}{t}\right)^j \widehat{u}^j \left(\frac{n}{t}\right) \\ &= \int_0^t \frac{(-1)^n}{n!} \left(\frac{n}{s}\right)^{n+1} \widehat{u}^{(n)} \left(\frac{n}{s}\right) \mathrm{d}s. \end{aligned}$$

By applying (9) to U and $\widehat{U}$ and by using (1.8) in [12], it follows that

$$E_1(n,t,U) := \left\| \int_0^t \frac{(-1)^n}{n!} \left(\frac{n}{s}\right)^{n+1} \widehat{u}^{(n)} \left(\frac{n}{s}\right) \mathrm{d}s - \int_0^t u(s)\,\mathrm{d}s \right\| \leq 2t \frac{1}{\sqrt{n}} \|u\|_\infty.$$

Thus, for all $u \in \mathcal{C}_b(\mathbb{R}^+, X)$, the Post-Widder inversion (10) converges "in the average" toward u at a rate of $\frac{1}{\sqrt{n}}$ (see also [13]). It is known (see, e.g.,[1, Thm. 1.7.7]) that the Post-Widder inversion (10) converges pointwise to $u(t)$ for all $u \in \mathcal{C}_{b,\omega}(\mathbb{R}^+, X)$ and all $t \geq 0$; however, the convergence can be arbitrarily slow.

3.2. Padé-{1,2} inversion ($m = 3$)

If $s = 2$, then $m = 3$ and the subdiagonal Padé approximation $r_{\{1,2\}}$ is given by

$$r(z) = \frac{6+2z}{6-4z+z^2} = \sum_{i=1}^{2} \frac{B_{\{1,i,1\}}}{b_i - z},$$

where $b_{1,2} = 2 \pm i\sqrt{2}$, $B_{\{1,1,1\}} = -1 + i\frac{5\sqrt{2}}{2}$, and $B_{\{1,2,1\}} = -1 - i\frac{5\sqrt{2}}{2}$. Now (4) holds for $B_0 = 0$, $r_i = 1$, and $B_{\{n,i,j\}}$ is obtained from (7) with $s = 2$. It follows that Theorem 6 holds for $m = 3$ and that

$$E_3(n,t,u) := \left\| \sum_{i=1}^{2} \sum_{j=1}^{n} B_{\{n,i,j\}} \left(\frac{n}{t}\right)^j \frac{(-1)^{j-1}}{(j-1)!} \widehat{u}^{(j-1)}\left(\frac{nb_i}{t}\right) - u(t) \right\| \tag{11}$$

satisfies the estimate

$$E_3(n,t,u) \le \begin{cases} C_3 t^k \frac{1}{n^{3k/4}} \|u^{(k)}\|_\infty & \text{if } u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X) \text{ and } 1 \le k \le 4, \\ C_3 \frac{1}{n^3} \|u\|_\infty & \text{if } u \in C_{ub}(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X) \end{cases}$$

for all $t \ge 0$. Moreover, $\lim_{n\to\infty} E_3(n,t,u) = 0$ for all $u \in \mathcal{C}_b(\mathbb{R}^+, X)$.

3.3. Radau IIA inversion ($m = 5$)

If $s = 3$, then $m = 5$ and the subdiagonal Padé approximant $r_{\{2,3\}}$ is given by

$$r(z) = \frac{3z^2 + 24z + 60}{-z^3 + 9z^2 - 36z + 60} = \sum_{i=1}^{3} \frac{B_{\{1,i,1\}}}{b_i - z},$$

where $b_1 = 3 - 3^{1/3} + 3^{2/3} \approx 3.63$, $b_{2,3} = 3 - \frac{1}{2}3^{2/3} + \frac{1}{2}3^{1/3} \pm \frac{1}{2}i\left(3^{5/6)} + 3^{7/6}\right) \approx 2.68 \pm 3.05i$ and $B_{\{1,i,1\}} = \frac{60+24b_i+3b_i^2}{\prod_{k\neq i}(b_k - b_i)}$. Now (4) holds for $B_0 = 0$, $r_i = 1$, and $B_{\{n,i,j\}}$ is given by (7) with $s = 3$. It follows that Theorem 6 holds for $m = 5$ and that

$$E_5(n,t,u) := \left\| \sum_{i=1}^{3} \sum_{j=1}^{n} B_{\{n,i,j\}} \left(\frac{n}{t}\right)^j \frac{(-1)^{j-1}}{(j-1)!} \widehat{u}^{(j-1)}\left(\frac{nb_i}{t}\right) - u(t) \right\| \tag{12}$$

satisfies the estimate

$$E_5(n,t,u) \le \begin{cases} C_5 t^k \frac{1}{n^{5k/6}} \|u^{(k)}\|_\infty & \text{if } u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X) \text{ and } 1 \le k \le 6, \\ C_5 \frac{1}{n^5} \|u\|_\infty & \text{if } u \in C_{ub}(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X) \end{cases}$$

for all $t \ge 0$. Moreover, for all $u \in \mathcal{C}_b(\mathbb{R}^+, X)$, $\lim_{n\to\infty} E_5(n,t,u) = 0$.

3.4. Padé-{3,4} inversion ($m = 7$)

The largest value of s for which all constants can be computed symbolically is $s = 4$. Then, $m = 7$ and the subdiagonal Padé approximation $r_{\{3,4\}}$ is given by

$$r(z) = \frac{4z^3 + 60z^2 + 360z + 840}{z^4 - 16z^3 + 120z^2 - 480z + 840} = \sum_{i=1}^{4} \frac{B_{\{1,i,1\}}}{b_i - z},$$

where the roots of $Q_{3,4}$ are given by $b_{1,2} \approx 3.213 \pm 4.773i$, $b_{3,4} \approx 4.787 \pm 1.567i$, and $B_{\{1,i,1\}} = \frac{4b_i^3+60b_i^2+360b_i+84}{\prod_{k\neq i}(b_k-b_i)}$. Now (4) holds for $B_0 = 0$, $r_i = 1$, and $B_{\{n,i,j\}}$ is given by (7) with $s = 3$. It follows that Theorem 6 holds for $m = 7$ and that

$$E_7(n,t,u) := \left\| \sum_{i=1}^{4} \sum_{j=1}^{n} B_{\{n,i,j\}} \left(\frac{n}{t}\right)^j \frac{(-1)^{j-1}}{(j-1)!} \widehat{u}^{(j-1)} \left(\frac{nb_i}{t}\right) - u(t) \right\| \qquad (13)$$

satisfies, for all $t \geq 0$,

$$E_7(n,t,u) \leq \begin{cases} C_7 t^k \frac{1}{n^{7k/8}} \|u^{(k)}\|_\infty & \text{if } u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X) \text{ and } 1 \leq k \leq 8, \\ C_7 \frac{1}{n^7} \|u\|_\infty & \text{if } u \in C_{ub}(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X). \end{cases}$$

Moreover, $\lim_{n\to\infty} E_7(n,t,u) = 0$ for all $u \in \mathcal{C}_b(\mathbb{R}^+, X)$.

Since the poles of r are given symbolically, all $4n$ coefficients $B_{\{n,i,j\}}$ ($1 \leq i \leq 4$, $1 \leq j \leq n$) needed in (13) are, in principal, computable symbolically (error free). However, since in applications it is often difficult to handle $\widehat{u}^{(j-1)}$ for large j (i.e., $j \geq 3$), let us consider (13) for $n = 2$. In this case, the eight coefficients $B_{\{2,i,j\}}$ ($1 \leq i \leq 4$, $1 \leq j \leq 2$) are easily computable

$$B_{\{2,i,1\}} = \sum_{\substack{j=1\\ j\neq i}}^{4} \frac{2B_{\{1,i,1\}}B_{\{1,j,1\}}}{b_j - b_i}, \qquad B_{\{2,i,2\}} = B_{\{1,i,1\}}^2,$$

and the 8-term inversion

$$E_7(2,t,u) := \left\| \sum_{i=1}^{4} \sum_{j=1}^{2} B_{\{2,i,j\}} \left(\frac{2}{t}\right)^j \frac{(-1)^{j-1}}{(j-1)!} \widehat{u}^{(j-1)} \left(\frac{2b_i}{t}\right) - u(t) \right\|. \qquad (14)$$

gives already reasonable results since $1/2^7 = 0.0078125$. In order to get better approximations while keeping the number of derivatives low, one has to increase the order m.

3.5. Padé-{10,11} inversion ($m = 21$)

If $s = 11$, then $m = 21$ and the subdiagonal Padé approximation $r_{\{10,11\}}$ is given by

$$r(z) = \frac{P(z)}{Q(z)} = \sum_{i=1}^{11} \frac{B_{\{1,i,1\}}}{b_i - z},$$

where P with $deg(P) = 10$ and Q with $deg(Q) = 11$ are as in (1) and where the zeros b_i of Q are given by $b_{1,2} \approx 5.46 \pm 17.60i, b_{3,4} \approx 9.23 \pm 13.71i, b_{5,6} \approx 11.60 \pm 10.15i, b_{7,8} \approx 13.11 \pm 6.72i, b_{9,10} \approx 13.96 \pm 3.34i, b_{11} \approx 14.23$, and $B_{\{1,i,1\}} = \frac{P(b_i)}{\prod_{k\neq i}(b_k - b_i)}$. For $n = 2$, the 22 coefficients $B_{\{2,i,j\}}$ $(1 \leq i \leq 11, 1 \leq j \leq 2)$ can be computed to any degree of accuracy and are given by

$$B_{\{2,i,1\}} = \sum_{\substack{j=1\\ j\neq i}}^{11} \frac{2B_{\{1,i,1\}}B_{\{1,j,1\}}}{b_j - b_i}, \quad \text{and} \quad B_{\{2,i,2\}} = B^2_{\{1,i,1\}}.$$

Consider the 22-term inversion

$$E_{21}(2,t,u) := \left\| \sum_{i=1}^{11} \sum_{j=1}^{2} B_{\{2,i,j\}} \left(\frac{2}{t}\right)^j \frac{(-1)^{j-1}}{(j-1)!} \widehat{u}^{(j-1)}\left(\frac{2b_i}{t}\right) - u(t) \right\|. \tag{15}$$

Since $1/2^{21} \leq 0.0000005$, Theorem 6 gives reasonably good results for $n = 2$ since

$$E_{21}(2,t,u) \leq \begin{cases} C_{21} t^k \frac{1}{2^{21k/22}} \|u^{(k)}\|_\infty & \text{if } u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X) \text{ and } 1 \leq k \leq 22, \\ C_{21} \frac{1}{2^{21}} \|u\|_\infty & \text{if } u \in C_{ub}(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X). \end{cases}$$

Clearly, the choice of $m = 21$ was arbitrary; i.e., if $n = 2$ and the subdiagonal Padé inversion should have an approximation error $E(n,t,u)$ of order 10^{-N}, then m should be an odd number larger than $10N/3$.

4. Restricted Padé inversion of the Laplace transform

A second class of examples of rational Laplace transform inversion methods is provided by the $\mathcal{A}$-stable restricted Padé approximants $r_{\{1\}}$ (Crank-Nicolson, $m = 2$) and $r_{\{2\}}$ (Calahan, $m = 3$), where $r_{\{j\}}$ is defined as in (2) (for a discussion of $r_{\{3\}}$ $(m = 4)$ and $r_{\{5\}}$ $(m = 6)$, see [33]). In contrast to the subdiagonal Padé approximants with $m > 1$, these approximants have only one single real pole. Therefore, their associated Laplace transform inversion methods require the knowledge of $\widehat{u}(\lambda)$ at *real numbers* $\lambda > 0$.

4.1. Crank-Nicolson inversion ($m = 2$)

The Crank-Nicolson approximation

$$r(z) = \frac{2+z}{2-z} = -1 + \frac{4}{2-z}$$

is an $\mathcal{A}$-stable Padé approximation to the exponential function of order $m = 2$. Let $u_0 = \lim_{\lambda\to\infty} \lambda\widehat{u}(\lambda) = u(0)$. Since

$$r^n\left(\frac{t}{n}z\right) = \sum_{j=0}^{n} \binom{n}{j} (-1)^{n-j} 2^{2j} \left(\frac{n}{t}\right)^j \frac{1}{\left(\frac{2n}{t} - z\right)^j},$$

it follows from Theorem 6 that $E(n,t,u) :=$

$$\left\| (-1)^n u_0 + (-1)^{n-1} \sum_{j=1}^{n} \binom{n}{j} 4^j \left(\frac{n}{t}\right)^j \frac{1}{(j-1)!} \widehat{u}^{(j-1)} \left(\frac{2n}{t}\right) - u(t) \right\|$$

satisfies, for all $t \geq 0$,

$$E_2(n,t,u) \leq \begin{cases} C_2 t \frac{1}{\sqrt{n}} \|u^{(1)}\|_\infty & \text{if } u, u^{(1)} \in \mathcal{C}_b(\mathbb{R}^+, X), \\ C_2 t^k \frac{1}{n^{2k/3}} \|u^{(k)}\|_\infty & \text{if } u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X) \text{ and } 2 \leq k \leq 3, \\ C_2 \frac{1}{n^2} \|u^{(2)}\|_\infty & \text{if } u, u^{(2)} \in C_{ub}(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X). \end{cases}$$

For $u \in C_{ub}(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$ the results can be improved by using Hansbo's stabilization methods [15]; for $u, u^{(1)} \in \mathcal{C}_b(\mathbb{R}^+, X)$ the results can be improved by stabilizing the Crank-Nicolson scheme using the methods in [31].

4.2. Calahan inversion ($m = 3$)

The Calahan approximation

$$r(z) = B_1 + \frac{B_2}{1 - bz} + \frac{B_3}{(1 - bz)^2}$$

with $b = \frac{1}{6}(3 + \sqrt{3})$, $B_1 = 1 - \sqrt{3}$, $B_2 = 3(-1 + \sqrt{3})$, $B_3 = 3 - 2\sqrt{3}$ is an $\mathcal{A}$-stable restricted Padé approximation of e^z of order $m = 3$. Since

$$r^n \left(\frac{t}{n} z\right) = \sum_{j=0}^{n} \sum_{k=0}^{j} \binom{n}{j} B_1^{n-j} B_2^{j-k} B_3^k \binom{j}{k} \left(\frac{n}{bt}\right)^{k+j} \frac{1}{(\frac{n}{bt} - z)^{k+j}},$$

it follows from Theorem 6 that

$$E_3(n,t,u) := \left\| B_1^n u_0 + \sum_{j=1}^{n} \sum_{k=0}^{j} \binom{n}{j} \binom{j}{k} B_1^{n-j} B_2^{j-k} B_3^k \left(\tfrac{n}{bt}\right)^{j+k} \tfrac{(-1)^{j+k-1}}{(j+k-1)!} \widehat{u}^{(j+k-1)} \left(\tfrac{n}{bt}\right) - u(t) \right\|$$

satisfies

$$E_3(n,t,u) \leq \begin{cases} C_3 t^k \frac{1}{n^{3k/4}} \|u^{(k)}\|_\infty & \text{if } u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X) \text{ and } 1 \leq k \leq 4, \\ C_3 \frac{1}{n^3} \|u^{(3)}\|_\infty & \text{if } u, u^{(3)} \in C_{ub}(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X) \end{cases}$$

for all $t \geq 0$. Moreover, the stability of the Calahan scheme, see Remark 3–(vi), yields $\lim_{n\to\infty} E_3(n,t,u) = 0$ for all $u \in \mathcal{C}_b(\mathbb{R}^+, X)$.

5. Applications and numerical examples

In order to demonstrate the accuracy of the rational inversion formulas, we provide in this section some numerical examples. First we compare the rational Laplace transform inversion method with the quadrature method for a scalar problem of convolution type that was considered in [39]. Then, it will be shown how to approximate solutions of scalar differential-difference equations, including the case of neutral differential-difference equations where the quadrature method for inverting the Laplace transform cannot be applied, by using the rational inversion of the Laplace transform method. Finally, we show two applications to evolution equations by approximating solutions of the abstract Cauchy problem $u'(t) = Au(t), u(0) = x$ and the fractional abstract Cauchy problem in a general Banach space for generators A of C-regularized semigroups and analytic semigroups, respectively. The semigroup approach has shown to be very fruitful for solving partial differential equations (and evolution equations) by rewriting a PDE in the form of an abstract Cauchy problem, see for example [1,9,11,27], or [38]. All the numerical implementations arising from rational approximations to the exponential of order less or equal than seven were calculated analytically, while the ones of higher order use double precision arithmetic for the calculation of the associated coefficients of Theorem 6.

5.1. Comparison with quadrature methods in the scalar case

In [39], W. McLean, I. H. Sloan, and V. Thomée use the numerical inversion of the Laplace transform provided by quadrature methods developed in [42] and [43] in order to obtain time discretizations for certain parabolic integro-differential equations. Section 5.1 of [39] shows the error of the approximation by the numerical inversion of the Laplace transform via the quadrature method to the solution $u(t) = e^{-t}(\cos(t) - \sin(t))$ of the integro-differential equation of convolution type

$$u'(t) + 2u(t) + \int_0^t 2u(s)\,\mathrm{d}s = 0 \qquad \text{for } t > 0, \quad \text{with } u(0) = 1. \tag{16}$$

In this case, $\widehat{u}(\lambda) = \frac{\lambda}{\lambda^2+2\lambda+2}$. Table 1 and Table 2 of [39] shows that the numerical approximation provided by the quadrature method is superior to the one obtained by using a finite difference method. Figure 1 shows the logarithmic error of different approximations obtained by using subdiagonal Padé schemes as well as the logarithmic error obtained when using the approximation by quadrature methods $U80$ to the solution u of (16).

In this case, the approximation of u by using the Padé-$\{20, 21\}$ scheme obtains more than 30 decimal places of accuracy on the interval $[0, 4]$ by adding 21 terms of the form $B_i\widehat{u}\left(\frac{t}{b_i}\right)$. Notice that this strongly suggests that the constants $C_m \to 0$ as $m \to \infty$.

5.2. First-order linear differential-difference equations of retarded and neutral type

In order to show examples where the accuracy of the rational inversion of the Laplace transform is time-dependent, we consider first-order linear differential-difference equations of retarded type. For referencesand a comprehensive introduction

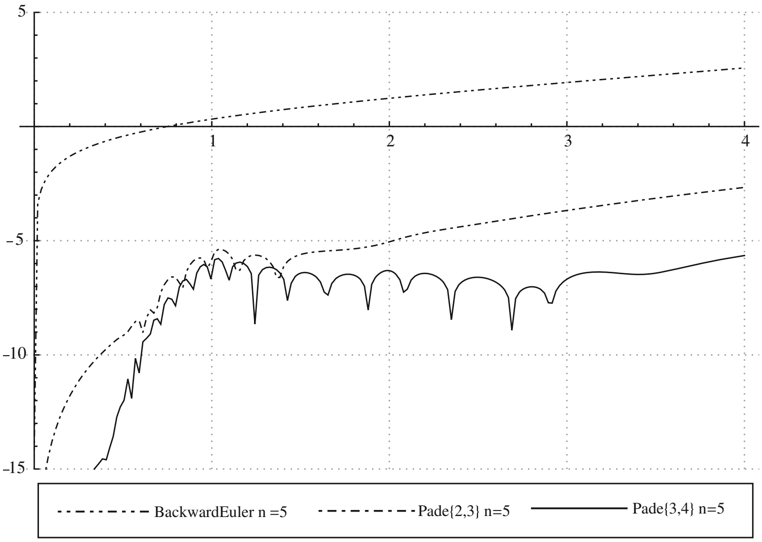

Figure 2. Logarithmic error $\log_{10}(E(n, t, u))$ for different schemes provided by Padé approximants for the approximation of the solution u of (17) for $t \in [0, 4]$

to differential-difference equations, see [4]. Let u be the solution of the differential-difference equation of retarded type given by

$$\begin{aligned} u'(t) &= u(t-1) \qquad t > 0 \\ u(t) &= g(t) \qquad t \in [-1, 0], \end{aligned} \tag{17}$$

where $g \in C([-1, 0], \mathbb{R})$. Under suitable conditions on g, one obtains that the unique solution u of (17) is k-times continuously differentiable on $[-1, \infty)$, see Thm. 3.1 of [4]. Clearly, the solution of (17) can be obtained by recursively integrating (17) on the intervals of the form $[n, n+1]$ for $n \in \mathbb{N}_0$. Furthermore, it can be shown that

$$\widehat{u}(\lambda) = \frac{e^{-\lambda} \int_{-1}^{0} e^{-\lambda s} g(s)\, \mathrm{d}s + g(0)}{\lambda - e^{-\lambda}} \qquad \text{for } \mathrm{Re}(\lambda) > 0. \tag{18}$$

Figure 2 shows the logarithmic error of the numerical approximation of the solution u of (17) by the rational inversion of the Laplace transform with $g(t) = \frac{1}{40320}(t^8 + 84t^6 + 616t^5 + 5950t^4 + 41384t^3 + 219268t^2 + 773128t + 1363209)$. In this case, $u \in C^8([-1, \infty), \mathbb{R})$ but $u \notin C^9([-1, \infty), \mathbb{R})$. Therefore, we can use rational approximations to the exponential up to order $m = 7$.

As a second example, consider the neutral delay differential equation

$$\begin{aligned} u'(t) &= u'(t-1) \qquad t > 0 \\ u(t) &= g(t) \qquad t \in [-1, 0], \end{aligned} \tag{19}$$

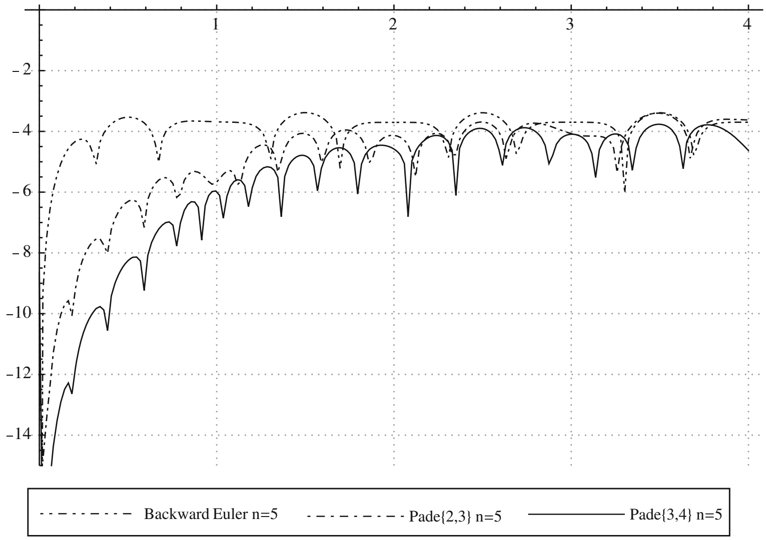

Figure 3. Logarithmic error $\log_{10}(E(n, t, u))$ for different schemes provided by Padé approximants for the approximation of the solution u of (19) for $t \in [0, 4]$

where $g \in C([-1, 0], \mathbb{R})$. In this case the solution u of (19) is simply the periodic extension of g over the intervals of the form $[n, n+1]$ for $n \in \mathbb{N}_0$ and under suitable conditions over g, $u \in C^k([-1, \infty))$. Furthermore, if $g(-1) = g(0)$ then

$$\widehat{u}(\lambda) = \frac{e^{-\lambda} \int_{-1}^{0} e^{-\lambda s} g(s)\, \mathrm{d}s}{1 - e^{-\lambda}} \qquad \text{for } \mathrm{Re}(\lambda) > 0. \tag{20}$$

Figure 3 shows the logarithmic error of the numerical approximation to the solution u of (19) by rational inversion of the Laplace transform with $g(t) = -6t^{14} - 42t^{13} - 125t^{12} - 204t^{11} - 195t^{10} - 106t^9 - 27t^8 + t^6$. In this case, $u \in C^8([-1, \infty), \mathbb{R})$ but $u \notin C^9([-1, \infty), \mathbb{R})$. Therefore, we can consider rational approximations to the exponential up to order $m = 7$.

REMARK 8. The quadrature methods for inverting the Laplace transform cannot be applied to solutions u of neutral differential-difference equations, since in this case the Laplace transform $\widehat{u}$ has infinitely many poles on a vertical line (as in (20)) and therefore there is no analytic extension of $\widehat{u}$ into a sectorial region $\{\lambda : |\arg(\lambda)| < \theta\}$ of angle $\theta > \frac{\pi}{2}$.

5.3. Approximating solutions of the abstract Cauchy problem

Time discretization methods for evolution equations of convolution type provided by the quadrature inversion method have shown to be very fruitful, see [32,42,43,45,46]. In order to show how to apply Theorem 6 for the approximation of solutions of the abstract Cauchy problem, we consider the theory of C-regularized semigroups. Let C be a bounded and injective operator defined on X. A strongly continuous map $W : [0,\infty) \to \mathscr{L}(X)$ is called a *C-regularized semigroup* or *C-semigroup* if $W(0) = C$ and $W(t)W(s) = CW(t+s)$ for all $t, s \geq 0$. A linear operator $B : D(B) \subseteq X \to X$ is called the generator of W if $Bx = C^{-1}\lim_{t\to 0}\frac{W(t)x - Cx}{t}$, where $D(B)$ denotes the maximal domain of B in X. A C-semigroup W is said to be of type (M,ω) if there exist $M \geq 1$ and $\omega \in \mathbb{R}$ such that $\|W(t)\|_{\mathscr{L}(X)} \leq Me^{\omega t}$ for all $t \geq 0$. Theorem 3.4 of [9] asserts that if W is a C-regularized semigroup generated by B, $x \in D(B)$ and $t \geq 0$, then $W(t)x = Cx + \int_0^t BW(s)x\,\mathrm{d}s$. In this way, $u(t) := W(t)x$ is a classical solution of the abstract Cauchy problem

$$(\mathrm{ACP}_C)\begin{cases} u'(t) = Bu(t), \\ u(0) = Cx. \end{cases}$$

Moreover, if $x \in D(B^k)$ for some $k \in \mathbb{N}$, then $u(t) := W(t)x \in C^k([0,\infty), X)$, and $u^{(k)}(t) = B^k u(t)$. The concept of C-semigroups is a natural extension of strongly continuous semigroups since a strongly continuous semigroup is an I-regularized semigroup where I is the identity operator on X. Furthermore, it allows the study of well-posed and ill-posed abstract Cauchy problems, see [9]. Generators of C-regularized semigroups include generators of integrated semigroups as well as distributional semigroups with important examples such as the Schrödinger operator $\Delta - V$ on $L^p(\mathbb{R}^N)$ for $1 \leq p \leq \infty$ for suitable potentials V, see [21] and [37]. It can be shown that if B is the generator of a C-regularized semigroup W of type (M,ω) then the C-resolvent set defined by $\rho_C(B) := \{\lambda \in \mathbb{C} : (\lambda - B)$ is injective and $\mathrm{Im}(C) \subseteq \mathrm{Im}(\lambda - B)\}$ is not empty. Furthermore, $\{\lambda : \mathrm{Re}(\lambda) > \omega\} \subseteq \rho_C(B)$, the map $\lambda \to R(\lambda, B)C := (\lambda - B)^{-1}C$ is holomorphic from $\mathrm{Re}(\lambda) > \omega$ into $\mathscr{L}(X)$, and the Laplace transform of W satisfies that $\widehat{W}(\lambda) = R(\lambda, B)C$ for $\lambda > \omega$, see [9, Prop. 17.2]. In this way, the approximation of solutions of $(\mathrm{ACP})_C$ when B generates a C-regularized semigroup as discussed in Theorem 3.1 of [20] can be obtained directly by applying Theorem 6 (iii) without the need of a functional calculus for generators of C-regularized semigroups. An important example is given by the Backward Euler scheme, i.e., $r(z) = \frac{1}{1-z}$ for $\mathrm{Re}(z) \leq 0$. Theorem 6(iii) asserts that if A generates a C-regularized semigroup of type (M,ω), then

$$W(t)x = \lim_{n\to\infty} R\left(1, \frac{t}{n}A\right)Cx = \lim_{n\to\infty}\frac{n}{t}R\left(\frac{n}{t}, A\right)Cx \qquad \text{for all } x \in X, \quad (21)$$

where the limit is uniform on compact sets and is $O(e^{\omega t}\frac{t}{\sqrt{n}})$ as $n \to \infty$ for $x \in D(A)$. Notice that if A generates a strongly continuous semigroup, then formula (21) becomes Hille's celebrated exponential formula.

As an example in which the solution has values in a Banach space, consider the first-order hyperbolic partial differential equation given by

$$\begin{aligned}\frac{\partial v}{\partial t}(t,w)+\frac{\partial v}{\partial w}(t,w)&=0 \qquad w\in(0,1),\\ v(t,0)&=0 \qquad t\geq 0,\\ v(0,w)&=f(w) \qquad w\in(0,1).\end{aligned} \tag{22}$$

Let $X := C_0(0,1)$ the space of continuous functions vanishing at $r = 0$ with the sup-norm (or $X = L^1(0,1)$ or $X = L^2(0,1)$). It is not hard to show that if $Af := -\frac{df}{dw}$ for $f \in \mathrm{Dom}(A)$, then A generates a strongly continuous semigroup T on X (the right shift semigroup), where $\mathrm{Dom}(A) := \{f \in X : f$ is absolutely continuous on $[0,1]$ with $f' \in X$ and $f(0) = 0\}$. Therefore, $u(t) := T(t)f \in C_b(\mathbb{R}^+, C_0(0,1))$ (or $C_b(\mathbb{R}^+, L^1(0,1))$ or $C_b(\mathbb{R}^+, L^2(0,1))$) satisfies that $u'(t) = Au(t)$ and $u(0) = f$ from which one obtains that the solution of (22) is given by $v(t,w) := T(t)f(w)$. Moreover,

$$R(\lambda,A)f(w)=\int_0^w e^{-\lambda(w-y)}f(y)\,\mathrm{d}y \quad \text{for } w\in(0,1) \text{ and } \mathrm{Re}(\lambda)\geq 0. \tag{23}$$

Since $\widehat{u}(\lambda) = \widehat{T}(\lambda)f = R(\lambda,A)f$, it follows that $\widehat{u}^{(j-1)}(\lambda) = R(\lambda,A)^j f$. If we denote $e_\lambda(w) := e^{-\lambda w}$, $(f * g)(w) := \int_0^w f(w-y)g(y)\,\mathrm{d}y$, and the nth convolution power by $g^{*n} := g * g * \cdots * g$ (n-times), then $\widehat{u}^{(j-1)}(\lambda) = e_\lambda^{*j} * f$. Theorem 6 asserts that if we consider the Subdiagonal Padé approximants of order $m = 2s-1$ given by (7), then

$$v(t,w)=\lim_{n\to\infty}\sum_{i=1}^{s}\sum_{j=1}^{n}B_{\{n,i,j\}}\left(\frac{n}{t}\right)^j\frac{(-1)^{j-1}}{(j-1)!}e^{*j}_{\frac{nb_i}{t}}*f(w), \tag{24}$$

where the limit is in the sup-norm (L^1 or L^2 norm resp.) with the corresponding error estimates for smooth initial data and where the norm of the error is in the sense of the sup-norm (L^1 or L^2 norm resp.). Figure 4 shows the logarithmic error of the approximation (24) to the solution u of (22) if $f(w) = \sin(\pi w)$ with $t \in [0,5]$ and $0 \leq w \leq 1$ for the Backward Euler and Padé-{2, 3} schemes.

5.4. Approximating solutions of the fractional abstract Cauchy problem

Let $\alpha \in (0,1)$. The fractional abstract Cauchy problem

$$\begin{aligned}D_t^\alpha u(t)&=\mathbb{A}u(t)\\ u(0)&=x,\end{aligned} \tag{25}$$

where D_t^α denotes the Caputo fractional derivative was studied by A. Kochubei in [22] and [23]. If $\mathbb{A}$ generates a strongly continuous semigroup of type (M,ω), then (25) has a unique solution u for which $\widehat{u}(\lambda) = \lambda^{\alpha-1}R(\lambda^\alpha,\mathbb{A})x$ for $\mathrm{Re}(\lambda) > \omega$, see [3, Corollary 2.10]. It follows from Theorem 6-(iv) that if r is a subdiagonal Padé approximant of order $m = 2s-1$, then

$$\lim_{n\to\infty}\sum_{i=1}^{s}\sum_{j=1}^{n}B_{\{n,i,j\}}\left(\frac{n}{t}\right)^j\frac{(-1)^{j-1}}{(j-1)!}\frac{d^{j-1}}{d\lambda^{j-1}}\left[\lambda^{\alpha-1}R(\lambda^\alpha,\mathbb{A})\right]\Big|_{\lambda=\frac{nb_i}{t}}x=u(t), \tag{26}$$

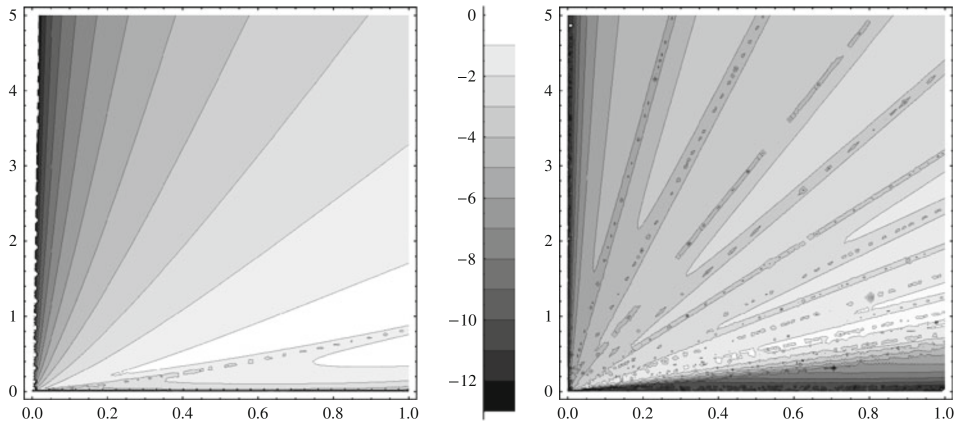

Figure 4. Contour plot of the Logarithmic error $\log_{10}(E(n,t,u))$ for the approximation (24) to the solution u of (22) if $f(w) = \sin(\pi w)$ with $t \in [0, 5]$ and $0 \leq w \leq 1$ for the Backward Euler (*left*) and Padé-{2, 3} (*right*) schemes with $n = 5$

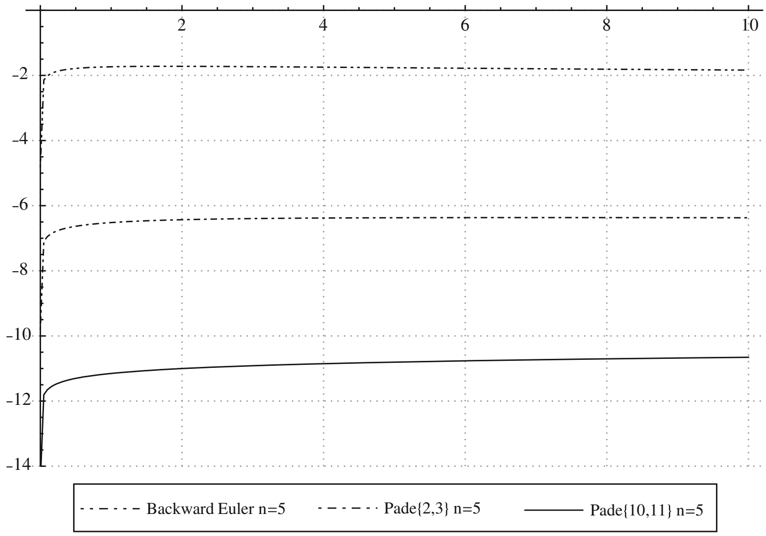

Figure 5. Logarithmic error $\log_{10}(E(n,t,u))$ for the approximation (26) to the solution v of (27) for $t \in [0, 10]$ with $\| \cdot \|_{L^2(0,\pi)}$

where the limit is uniform on compact sets and where the error is given by Theorem 6-(iii). In this way, (26) provides a new method for the approximation of solutions of the fractional abstract Cauchy problem (25).

A classical example where the solution can be explicitly found is provided by the fractional diffusion equation on the Hilbert space $X := L^2(0, \pi)$ given by

$$\begin{aligned} D_t^{\frac{1}{2}} v(t, w) &= \frac{\partial^2}{\partial w^2} v(t, w) \qquad 0 < w < \pi, \quad t > 0 \\ v(0, w) &= \sin(w) \qquad 0 < w < \pi \\ v(t, 0) &= 0 = v(t, \pi) \qquad t > 0. \end{aligned} \tag{27}$$

In this case, if $\mathbb{A} f := f''$ (the second derivative) with $D(\mathbb{A}) := \{f \in H^2(0, \pi) : f(0) = 0 = f(\pi)\}$, then $\mathbb{A}$ generates an analytic semigroup $S(t)$ on $X = L^2(0, \pi)$ for which $u(t) := S_{\frac{1}{2}}(t)x \in C_{ub}(\overline{\Sigma_\theta}, L^2(0, \pi)) \cap H(\Sigma_\theta, L^2(0, \pi))$ satisfies that $D_t^{\frac{1}{2}} u(t) = \mathbb{A} u(t)$ where $x = \sin(\cdot)$, see [3, Corollary 2.17]. Thus, (27) is equivalent to (25) with $\alpha = \frac{1}{2}$. Therefore, the solution $v(t, w) = e^t \operatorname{erfc}(\sqrt{t}) \sin(w)$ of (27) can be approximated uniformly in time by (26) where the limit is in the L^2-sense and the error norm is in the sense of L^2 as well. Figure 5 shows the logarithmic error for the approximation (26) to the solution of (27) when using some of the schemes of Sect. 3.

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