RATIONAL APPROXIMATIONS OF SEMIGROUPS WITHOUT SCALEING AND SQUARING

FRANK NEUBRANDER
Department of Mathematics, Louisiana State University
Baton Rouge, LA 70803, USA

KORAY ÖZER
Department of Mathematics, Roger Williams University
Bristol, RI 02809, USA

TERESA SANDMAIER
Mathematisches Institut, Universität Tübingen
Tübingen, 72076, Germany

Abstract. We show that for all $q \geq 1$ and $1 \leq i \leq q$ there exist pairwise conjugate complex numbers $b_{q,i}$ and $\lambda_{q,i}$ with $\text{Re}(\lambda_{q,i}) > 0$ such that for any generator $(A, D(A))$ of a bounded, strongly continuous semigroup $T(t)$ on Banach space $X$ with resolvent $R(\lambda, A) := (\lambda I - A)^{-1}$ the expression $b_{q,1} t R(\lambda_{q,1}, A) + b_{q,2} t R(\lambda_{q,2}, A) + \cdots + b_{q,q} t R(\lambda_{q,q}, A)$ provides an excellent approximation of the semigroup $T(t)$ on $D(A^{2q-1})$. Precise error estimates as well as applications to the numerical inversion of the Laplace transform are given.

1. Introduction. In this paper we prove a new variant of the following key result on the approximation of strongly continuous semigroups (see [5]).

Theorem 1.1. (Hersh-Kato, Brenner-Thomée). Let $r$ be an $A$-stable rational approximation scheme of the exponential of order $m$ and $(A, D(A))$ be the generator of a strongly continuous semigroup $T(t)$ of type $(M,0)$. Then there exists a constant $C$ depending solely on $r$ such that

$$
\| r(\frac{t}{n} A)^n x - T(t)x \| \leq MC t^{m+1} \frac{1}{n^m} \| A^{m+1} x \|
$$

for all $n \in \mathbb{N}, t \geq 0$, and $x \in D(A^{m+1})$.

A slightly less sharp result appeared first in a 1979 paper of Reuben Hersh and Tosio Kato in the SIAM Journal of Numerical Analysis [7]. In the same issue, Philip Brenner and Vidar Thomée [3] could weaken the regularity assumptions and show the theorem as stated above. In this paper, they also found error estimates for $\| r(\frac{k}{n} A)^n x - T(t)x \|$ for $x \in D(A^k)$, where $0 \leq k \leq m + 1$. In 2007, this result was again improved by Mihály Kovács [11] giving error estimates for $x \in F$, where $F$ are interpolation spaces between $D(A^{m+1})$ and $X$. In all these contributions, no estimates are provided for the constant $C$. This is being done in the dissertation of

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William Harrison [6] for the case where \( r \) is an \( \mathcal{A} \)-stable rational \( \text{Padé} \)-approximation of the exponential or order \( m \). To keep the presentation of the material as readable as possible, we consider here mainly subdiagonal rational \( \text{Padé} \)-approximations \( r_m \) of order \( m \) and highlight the case \( n = 1 \). In particular, we will show that there are constants \( C_m \) which are rapidly decreasing to zero as \( m \to \infty \) such that

\[
\| r_m(tA)x - T(t)x \| \leq MC_m e^{m+1}\|Ax^{m+1}\|
\]

for all \( t \geq 0 \) and \( x \in D(A^{m+1}) \).

2. Preliminaries. 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 \( p := \text{deg}(P) \leq \text{deg}(Q) \), and

(i) \( |r(z) - e^z| \leq C_m|z|^{m+1} \) for \( |z| \) sufficiently small, and

(ii) \( r(\lambda) \leq 1 \) for \( \text{Re}(\lambda) \leq 0 \).

It is a well-known result of Padé [14] 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 \( r = \frac{P(z)}{Q(z)} \), where

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

Moreover, for every Padé approximation \( r(z) = \frac{P(z)}{Q(z)} \) of the exponential of order \( m = p + q \) we have that

\[
r(z) - e^z = \frac{(-1)^{q+1}}{Q(z)} \frac{1}{m!} z^{m+1} e^z \int_0^1 s^p (1-s)^q e^{-sz} ds
\]

(see, for example, [15], Section 75 (Die Exponentialfunktion), or [18]). As shown in [4], Padé approximations are \( \mathcal{A} \)-stable if and only if \( q - 2 \leq p \leq q \). A rational \( \text{Padé} \) approximation \( r(z) = \frac{P(z)}{Q(z)} \) is called subdiagonal if \( p = q - 1 \). In particular, a subdiagonal Padé approximation is always \( \mathcal{A} \)-stable, of odd approximation order \( m = 2q - 1 = 2p + 1 \), and the polynomial \( Q(z) \) has \( q \) distinct roots \( \lambda_i \) with \( \text{Re}(\lambda_i) > 0 \) such that

\[
Q(z) = \sum_{j=0}^{q} \frac{(m-j)!q!}{m!j!(q-j)!} (-1)^j = c(\lambda_1 - z) \cdot \ldots \cdot (\lambda_q - z)
\]

where \( c = \frac{(m-q)!}{m!} = \frac{p!}{m!} \). Moreover, if \( q \) is even, then all roots \( \lambda_i \) are pairwise complex conjugates, and if \( q \) is odd the the largest root \( \lambda_q \) is real and all the other roots pairwise complex conjugates. In particular,

(i) \( \lambda_1 \cdot \lambda_2 \cdot \ldots \cdot \lambda_q = |\lambda_1| \cdot |\lambda_2| \cdot \ldots \cdot |\lambda_q| = \frac{p!}{m!} \)

(ii) \( (\text{Re}(\lambda_1) \cdot \ldots \cdot \text{Re}(\lambda_q))^{1/q} \leq \frac{\text{Re}(\lambda_1) + \ldots + \text{Re}(\lambda_q)}{q} = p + 1 \)

If \( q \leq 15 \) and \( q - 2 \leq p \leq q \), then \( p \leq (\text{Re}(\lambda_1) \cdot \ldots \cdot \text{Re}(\lambda_q))^{1/q} \). If \( 16 \leq q \leq 28 \) and \( q - 2 \leq p \leq q \), then \( p - 1 \leq (\text{Re}(\lambda_1) \cdot \ldots \cdot \text{Re}(\lambda_q))^{1/q} \). For a proof, see [18]. Finally, a subdiagonal Padé approximation \( r(z) = \frac{P(z)}{Q(z)} \) has the representation

\[
r(z) = \frac{P(z)}{Q(z)} = \frac{b_1}{\lambda_1 - z} + \frac{b_2}{\lambda_2 - z} + \ldots + \frac{b_q}{\lambda_q - z}.
\]
where
\[ b_t := \frac{P(\lambda_i)}{\prod_{j=1}^{m}(\lambda_j - \lambda_i)}. \]

In particular, if \( r \) is a subdiagonal Padé approximation of order \( m = 2q - 1 \) and if \( A \) is the generator of a bounded strongly continuous \( T(t) \), then it follows from the Hille-Phillips functional calculus that for all \( t > 0 \)
\[ r(tA) = \frac{P(tA)}{Q(tA)} = \frac{b_1}{t} R(\frac{\lambda_1}{t}, A) + \frac{b_2}{t} R(\frac{\lambda_2}{t}, A) + \cdots + \frac{b_q}{t} R(\frac{\lambda_q}{t}, A). \]  
(2)

3. Approximations of semigroups without scaling and squaring. We now come to the main result of this paper. Our goal is to approximate semigroups \( T(t) \) in terms of sums of resolvents of the form (2), where \( r \) is an appropriately chosen subdiagonal Padé approximation of order \( m = 2q - 1 \).

**Theorem 3.1.** Let \( r = \frac{P}{Q} \) be a subdiagonal Padé approximation scheme of the exponential of order \( m \) given by (1) and \( (A, D(A)) \) be the generator of a strongly continuous semigroup \( T(t) \) of type \((M, 0)\). Then
\[ \|r(tA)x - T(t)x\| \leq MC_m t^{m+1} \|A^{m+1}x\| \]
for all \( t \geq 0 \) and \( x \in D(A^{m+1}) \) where
\[ C_m = \frac{2\sqrt{\pi}}{p!} \frac{1}{\prod \text{Re}(\lambda_i) \cdots \text{Re}(\lambda_q)} \left[ \frac{(2p)! (2q)!}{(2p + 2q + 1)!} \right]^{\frac{1}{2}} \left( \sum_{k=1}^{q} \frac{1}{\text{Re}(\lambda_k)} \right)^2 + \frac{(2p + 2q + 3)(2p + 2q + 2)}{2p + 2q + 3} \]
and \( \lambda_i \) are the zeros of the polynomial \( Q \).

For \( m \in \{1, 3, 5, 7, \cdots, 47\} \) the constants \( C_m \) are \( C_1 \leq 2.111 \times 10^0, C_3 \leq 9.034 \times 10^{-2}, C_5 \leq 1.492 \times 10^{-5}, C_7 \leq 1.257 \times 10^{-5}, C_9 \leq 6.386 \times 10^{-8}, C_{11} \leq 2.165 \times 10^{-10}, C_{13} \leq 5.245 \times 10^{-13}, C_{15} \leq 9.626 \times 10^{-16}, C_{17} \leq 1.345 \times 10^{-18}, C_{19} \leq 1.519 \times 10^{-21}, C_{21} \leq 1.403 \times 10^{-24}, C_{23} \leq 1.079 \times 10^{-27}, C_{25} \leq 7.024 \times 10^{-31}, C_{27} \leq 3.917 \times 10^{-34}, C_{29} \leq 1.893 \times 10^{-37}, C_{31} \leq 8.000 \times 10^{-41}, C_{33} \leq 2.983 \times 10^{-44}, C_{35} \leq 9.887 \times 10^{-48}, C_{37} \leq 2.931 \times 10^{-51}, C_{39} \leq 7.821 \times 10^{-55}, C_{41} \leq 1.888 \times 10^{-58}, C_{43} \leq 4.141 \times 10^{-62}, C_{45} \leq 8.925 \times 10^{-66}, C_{47} \leq 1.522 \times 10^{-69}. \)

**Proof.** From the Hille-Phillips functional calculus it follows that
\[ r(tA)x - T(t)x = \int_{0}^{\infty} T(s)x d[\alpha - H_t](s), \]
where \( r(z) = \int_{0}^{\infty} e^{zs}d\alpha(s) \) for \( \text{Re}(z) \leq 0 \) and \( H_t \) is the normalized Heaviside function defined on \([0, \infty)\). Since \( \alpha(0) - H_t(0) = \alpha(\infty) - H_t(\infty) = 0 \), integration by parts yields that
\[ r(tA)x - T(t)x = -\int_{0}^{\infty} [\alpha - H_t](s) dT(s)x \]
for all \( x \in X \). If \( x \in D(A) \), then \( s \rightarrow T(s)x \) is continuously differentiable with \( \frac{dT}{ds}T(s)x = T(s)Ax \). Therefore, for \( x \in D(A), \)
\[ r(tA)x - T(t)x = -\int_{0}^{\infty} [\alpha - H_t](s)T(s)Ax ds. \]
For $1 \leq k \leq m$, let $I_k[\alpha - H_t](s)$ denote the $k$-th antiderivative of $\alpha - H_t$; i.e.,

$$I_k[\alpha - H_t](s) = \int_0^s \frac{(s-r)^{k-1}}{(k-1)!} [\alpha - H_t](r) \, dr.$$ 

It can be shown that

$$I_k[\alpha - H_t](0) = I_k[\alpha - H_t](\infty) = 0$$

for $1 \leq k \leq m$ (see [12] or [16], Lemma III.6). Thus for $1 \leq k \leq m$ and $x \in D(A^{k+1})$, $k$ consecutive integrations by parts give

$$r(t)x - T(t)x = (-1)^{k+1} \int_0^\infty I_k[\alpha - H_t](s) T(s) A^{k+1} x \, ds. \quad (3)$$

As a consequence of (3), one obtains

$$\|r(t)x - T(t)x\| = M \|A^{k+1} x\| \|I_k[\alpha - H_t]\|_{L(R^+)} \quad (4)$$

for $t \geq 0$ and $x \in D(A^{k+1})$. In order to estimate $\|I_k[\alpha - H_t]\|_{L^1(\mathbb{R}^+)}$, one may use the following Fourier representation of $I_k[\alpha - H_t]$ (for details, see [12] or [16], Lemma III.6):

$$I_k[\alpha - H_t](s) = \left( \frac{1}{t} \right)^{k+1} \frac{1}{\sqrt{2\pi}} \mathcal{F} \left[ \frac{r(it\cdot) - e^{it\cdot}}{i\cdot} \right] (s) \quad (5)$$

for all $s \in (0, \infty)$, where

$$\mathcal{F}[f](s) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty e^{-isv} f(v) \, dv.$$ 

From [16], the representation

$$r(-tz) - e^{-tz} = \int_0^\infty e^{-sz} \, d[\alpha - H_t](s) \quad (6)$$

exists for $\text{Re}(z) \geq 0$ where $\alpha - H_t \in NBV^0(0, \infty)$. Recall that the complex inversion formula (see [17], Chapter II, Theorem 7.6a) states that if $\alpha \in NBV^0(0, \infty)$ and $f(z) = \int_0^\infty e^{-sz} \, d\alpha(s)$ converges for all $\text{Re}(z) > \sigma_c$, then for $c > \max[\sigma_c, 0]$

$$\lim_{R \to \infty} \int_{c-iR}^{c+iR} \frac{f(z)}{z} e^{zs} \, dz = \begin{cases} \frac{\alpha(s)}{\alpha(0^+)} & : n > 0 \\ \frac{s}{2} & : s = 0 \\ 0 & : s < 0 \end{cases}.$$ 

Then it follows from (6) and the complex inversion formula that

$$\alpha(s) - H_t(s) = \frac{1}{2\pi i} \lim_{R \to \infty} \int_{c-iR}^{c+iR} \frac{r(-tz) - e^{-zt}}{z} e^{zs} \, dz.$$ 

Using the $A$-stability of $r$ as well as Cauchy’s Theorem, one obtains

$$\alpha(s) - H_t(s) = \frac{1}{2\pi i} \lim_{R \to \infty} \int_{-iR}^{iR} \frac{r(-tz) - e^{-zt}}{z} e^{zs} \, dz$$

$$= \frac{-1}{\sqrt{2\pi}} \mathcal{F} \left[ \frac{r(it\cdot) - e^{it\cdot}}{i\cdot} \right] (s). \quad (7)$$
With an induction argument, one can show that (7) implies (5) and thus
\[ \|I_m[\alpha - H_1]\|_{L^1(\mathbb{R}^+)} = \frac{1}{\sqrt{2\pi}} \|F \left[ \frac{r(it(\cdot)) - e^{it(\cdot)}}{(\cdot)^{m+1}} \right]\|_{L^1(\mathbb{R}^+)} \leq \frac{1}{\sqrt{2\pi}} \|F \left[ \frac{[e^{-i(\cdot)}r((\cdot))] - 1}{(\cdot)^{m+1}} \right]\|_{L^1(\mathbb{R})}. \]

Simple substitutions yield
\[ \|I_m[\alpha - H_1]\|_{L^1(\mathbb{R}^+)} \leq \frac{1}{\sqrt{2\pi}} t^{m+1} \|F[h]\|_{L^1(\mathbb{R})}, \]
where
\[ h(s) := \frac{[e^{-is}r(is)] - 1}{s^{m+1}} \]
for \( s \in \mathbb{R}. \) Recall that if \( f \in L^2(\mathbb{R}) \) and \( g : s \to sf(s) \in L^2(\mathbb{R}), \) then Carlson’s inequality implies that \( f \in L^1(\mathbb{R}) \) and
\[ \|f\|_{L^1(\mathbb{R})} \leq \sqrt{\pi} \|f\|_{L^2(\mathbb{R})} \|g\|_{L^2(\mathbb{R})}. \]
For an absolutely continuous function \( g \in L^2 \) with \( g' \in L^2, \) it is well known that
\[ isF[g] = F'[g](s) \]
almost everywhere. Thus, if \( f = F[g] \in L^2(\mathbb{R}) \) for some absolutely continuous \( g \in L^2(\mathbb{R}), \) Carlson’s inequality implies that
\[ \|F[g]\|_1^2 \leq \sqrt{\pi} \|F[g]\|_{L^2(\mathbb{R})} \|F[g']\|_{L^2(\mathbb{R})}. \]
Furthermore, Parseval’s identity, \( \|F[g]\|_{L^2} = \|g\|_{L^2} \) for \( g \in L^2(\mathbb{R}), \) shows that
\[ \|F[g]\|_1 \leq \sqrt{\pi} \|g\|_{L^2} \|g'\|_{L^2}. \]
Using these properties and inequalities, it follows from (8) that
\[ \|I_m[\alpha - H_1]\|_{L^1(\mathbb{R}^+)} \leq \frac{1}{\sqrt{2}} t^{m+1} \|F[h]\|_{L^2(\mathbb{R})} \|h\|_{L^2(\mathbb{R})} \|h'\|_{L^2(\mathbb{R})} \]
\[ = \frac{1}{\sqrt{2}} t^{m+1} \|h\|_{L^2(\mathbb{R})} \|h'\|_{L^2(\mathbb{R})}. \]
Now, returning to (4), we obtain
\[ \|r(tA)x - T(t)x\| \leq M \|A^{m+1}x\| \frac{1}{s^{m+1}} t^{m+1} \|h\|_{L^2(\mathbb{R})} \|h'\|_{L^2(\mathbb{R})}, \]
where
\[ h(s) = \frac{[e^{-is}r(is)] - 1}{s^{m+1}} = \frac{[e^{-is}r(is)] - 1}{(is)^{m+1}}. \]
It is advantageous to use the following representation due to O. Perron [15] (see also [18]):
\[ r(z) - e^z = \frac{(-1)^q+1}{Q(z)} \frac{1}{m!} z^{m+1} e^z \int_0^1 t^q(1-t)^q e^{-tz} dt \]
where \( z \in \mathbb{C} \) and \( z \neq \lambda_1, \ldots, \lambda_q. \) Thus
\[ \frac{e^{-z}r(z) - 1}{z^{m+1}} = \frac{(-1)^q+1}{Q(z)} \frac{1}{m!} \int_0^1 t^q(1-t)^q e^{-tz} dt, \]
and therefore
\[ h(s) = (-1)^q t^{m+1} \frac{1}{m!} Q(is) \int_0^1 t^p (1 - t)^q e^{-tis} dt. \]

In order to estimate \( h(s) \), we use that
\[ \frac{1}{Q(is)} = \frac{1}{c} \frac{1}{\lambda_1 - is} \cdots \frac{1}{\lambda_q - is} \]
with \( c = \frac{p!}{m!} \). Since
\[ |\lambda - is| \leq \sqrt{\text{Re}(\lambda)^2 + (\text{Im}(\lambda) - s)^2} \leq \frac{1}{\text{Re}(\lambda)} \]
it follows that
\[ \frac{1}{|Q(is)|} \leq \frac{m!}{p!} \frac{1}{\text{Re}(\lambda_1) \cdots \text{Re}(\lambda_q)}. \]

Thus
\[ |h(s)| \leq \frac{1}{p! \text{Re}(\lambda_1) \cdots \text{Re}(\lambda_q)} \left| \int_0^1 t^p (1 - t)^q e^{-tis} dt \right|. \]

Now
\[ \int_0^1 t^p (1 - t)^q e^{-tis} dt = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi_m(t) e^{-itis} d\tau = F(\Psi_m)(s) \]
with
\[ \Psi_m(t) := \sqrt{2\pi} \begin{cases} t^p (1 - t)^q & : 0 \leq t < 1 \\ 0 & : \text{else} \end{cases} \]

Then
\[ \left\| \int_0^1 t^p (1 - t)^q e^{-tis} dt \right\|_2 = \| F(\Psi_m) \|_2 = \| \Psi_m \|_2 \]
which means
\[ \left\| \int_0^1 t^p (1 - t)^q e^{-tis} dt \right\|_2^2 = \| F(\Psi_m) \|_2^2 = \| \Psi_m \|_2^2. \]

In order to estimate \( \| \Psi_m \|_2^2 \), the following representation of the Beta function from [1] (Section 11.21) is needed. For \( p, q > -1 \) and \( \Gamma(n + 1) = n! \),
\[ B(p + 1, q + 1) = \int_0^1 x^p (1 - x)^q dx = \frac{\Gamma(p + 1) \Gamma(q + 1)}{\Gamma(p + q + 2)}. \]

Then
\[ \| \Psi_m \|_2^2 = \int_{-\infty}^{\infty} |\Psi_m(t)|^2 d\tau = 2\pi \int_0^1 t^{2p} (1 - t)^{2q} dt = 2\pi \frac{(2p)! (2q)!}{(2p + 2q + 1)!} \]
which implies
\[ \left\| \int_0^1 t^p (1 - t)^q e^{-tis} dt \right\|_2^2 = \frac{2\pi (2p)! (2q)!}{(2p + 2q + 1)!}. \]

Returning to (3), it follows that
\[ |h(s)| \leq \frac{1}{p! \text{Re}(\lambda_1) \cdots \text{Re}(\lambda_q)} \left| \int_0^1 t^p (1 - t)^q e^{-tis} dt \right|. \]
which means that
\[
\| h \|_{L^2(\mathbb{R})}^2 \leq \left( \frac{1}{p!} \text{Re}(\lambda_1) \cdots \text{Re}(\lambda_q) \right)^2 \left\| \int_0^1 t^p (1 - t)^q e^{-tis} \, dt \right\|_2
\]

\[
= \left( \frac{1}{p!} \text{Re}(\lambda_1) \cdots \text{Re}(\lambda_q) \right)^2 \left[ 2\pi \frac{(2p)!(2q)!}{(2p + 2q + 1)!} \right].
\]

Hence,
\[
\| h \|_{L^2(\mathbb{R})} \leq \left( \frac{1}{p!} \text{Re}(\lambda_1) \cdots \text{Re}(\lambda_q) \right)^{\frac{1}{2}} \left[ 2\pi \frac{(2p)!}(2p + 2q + 1)! \right]^{\frac{1}{2}}.
\]

To estimate \( \| h' \|_2 \), notice that
\[
h'(s) = \frac{(-1)^q + 2i^m + 2}{m!} \left[ \frac{Q'(is)}{Q(is)} \int_0^1 t^p (1 - t)^q e^{-tis} \, dt \right].
\]

Let \( Q(z) = c(\lambda_1 - z) \cdots (\lambda_q - z) \), then \( Q'(z) = -c \sum_{k=1}^q (\prod_{j \neq k} (\lambda_j - z)) \) which implies \( \frac{Q'(z)}{Q(z)} = \sum_{k=1}^q \frac{1}{\lambda_k - z} \) and thus
\[
\left| \frac{Q'(is)}{Q(is)} \right| \leq \sum_{k=1}^q \frac{1}{|\lambda_k - is|} \leq \sum_{k=1}^q \frac{1}{\text{Re}(\lambda_k)}.
\]

Also recall that \( \frac{1}{|Q(is)|} \leq \frac{m!}{p! \text{Re}(\lambda_1) \cdots \text{Re}(\lambda_q)} \). Define
\[
c_1 := \left( \frac{1}{p!} \text{Re}(\lambda_1) \cdots \text{Re}(\lambda_q) \right)^2.
\]

It follows from \( |a + b|^2 \leq 2|a|^2 + 2|b|^2 \) that
\[
\| h' \|_2 \leq c_1 \int_{-\infty}^\infty \left[ 2 \left( \sum_{k=1}^q \frac{1}{\text{Re}(\lambda_k)} \right)^2 \left| \int_0^1 t^p (1 - t)^q e^{-tis} \, dt \right|^2 \right] \, ds
\]

\[
\leq c_1 \left[ 2 \left( \sum_{k=1}^q \frac{1}{\text{Re}(\lambda_k)} \right)^2 \left( \int_0^1 t^p (1 - t)^q e^{-tis} \, dt \right)^2 + 2 \left( \int_0^1 t^{p+1} (1 - t)^q e^{-tis} \, dt \right)^2 \right] \, ds
\]

\[
\leq c_1 \left[ 2 \left( \sum_{k=1}^q \frac{1}{\text{Re}(\lambda_k)} \right)^2 \left( 2\pi \frac{(2p)!(2q)!}{(2p + 2q + 1)!} + 2 \frac{(2p + 2)!(2q)!}{(2p + 2q + 3)!} \right) \right]
\]

\[
= c_1 c_2
\]

where
\[
c_2 := 4\pi \left[ \left( \sum_{k=1}^q \frac{1}{\text{Re}(\lambda_k)} \right)^2 \left( \frac{(2p)!}{(2p + 2q + 1)!} + \frac{(2p + 2)!}{(2p + 2q + 3)!} \right) \right]
\]

and thus
\[
\| h' \|_2 \leq \left( \frac{1}{p!} \text{Re}(\lambda_1) \cdots \text{Re}(\lambda_q) \right)^{\frac{1}{2}} c_2^{\frac{1}{2}}.
\]

Now
\[
\| h \|_{L^2(\mathbb{R})} \| h' \|_{L^2(\mathbb{R})} \leq \left( \frac{1}{p!} \text{Re}(\lambda_1) \cdots \text{Re}(\lambda_q) \right) \left[ 2\pi \frac{(2p)!}{(2p + 2q + 1)!} \right]^{\frac{1}{2}} c_2^{\frac{1}{2}}.
\]
Since

\[
c_{2}^{-\frac{1}{2}} = \left[4\pi \left(\frac{(2p)!}{(2p+2q+1)!}\right)^{\frac{1}{2}} \left(\sum_{k=1}^{\infty} \frac{1}{\text{Re}(\lambda_k)}\right)^{2} + \frac{(2p+2)(2p+1)}{(2p+2q+3)(2p+2q+2)}\right]^{\frac{1}{4}},
\]

it follows that

\[
\|h\|_{L^2(\mathbb{R})} \|h^\prime\|_{L^2(\mathbb{R})} \leq \frac{1}{\sqrt{p!}} \frac{1}{\text{Re}(\lambda_1) \cdots \text{Re}(\lambda_q)} 2\sqrt{\pi} \left[\left(\frac{(2p)!}{(2p+2q+1)!}\right)^{\frac{1}{4}} \left(\sum_{k=1}^{\infty} \frac{1}{\text{Re}(\lambda_k)}\right)^{2}\right]^{\frac{1}{4}} \left(\frac{(2p+2)(2p+1)}{(2p+2q+3)(2p+2q+2)}\right)^{\frac{1}{4}}.
\]

Now the claim follows from (9).

If \(0 \leq k \leq m-1\), the previous proof can be modified to get estimates for constants \(C_{m,k}\) such that

\[
\|r(tA)x - T(t)x\| \leq MC_{m,k}^{k+1}\|A^{k+1}x\|
\]

for all \(t \geq 0\) and \(x \in D(A^{k+1})\) (see [6]). As long as \(q = m - p \leq k < m\), the constants \(C_{m,k}\) still converge rapidly to zero as \(m\) gets larger, although the speed of convergence slows down with decreasing \(k\). If \(k < q\), then the situation becomes less clear and it remains an open problem whether or not there is a sequence \(r_m\) of rational Padé approximations \(r_m\) such that

\[
r_m(tA)x \to T(t)x \quad \text{as} \quad m \to \infty
\]

uniformly on compacts for all \(x \in D(A)\).

In order to translate Theorem 3.1 into the language of Laplace transforms, the following remark is useful.

**Proposition 1.** (Transference Principle.) Let \(X\) be a Banach space, \(f \in C_0([0,\infty), X)\) with Laplace transform \(\hat{f}(\lambda) = \int_0^\infty e^{-\lambda t} f(t)\, dt\) for \(\text{Re}(\lambda) > 0\), and let \(A\) be the generator of a bounded, strongly continuous semigroup \(T(t)\) on some Banach space \(Z\) with resolvent \(R(\lambda, A)\) for \(\text{Re}(\lambda) > 0\). Then the following three problems are equivalent.

(I) Compute \(f(t)\) in terms of \(\hat{f}(\lambda)\).

(II) Compute \(T(t)z\) in terms of \(R(\lambda, A)z\) for all \(z \in Z\).

(III) Let \(A = \frac{d}{dt}\) on \(F = C_0([0,\infty), X)\). Compute the shift semigroup \(T(t)f = f(t+\cdot)\) in terms of \(R(\lambda, A)f(\cdot)\) for all \(f \in F\).

**Proof.** The implication (I) \(\implies\) (II) follows from the fact that \(t \to T(t)z \in C_0([0,\infty), Z)\) and \(R(\lambda, A)z = \int_0^\infty e^{-\lambda t} T(t)z\, dt\) for all \(z \in Z\); i.e., the resolvent of the operator \(A\) is the Laplace transform of the operator semigroup \(T(t)\) (see [2], [5]). The implication (II) \(\implies\) (III) holds because (a) the shift semigroup is bi-continuous with generator \(A = \frac{d}{dt}\) on \(F = C_0([0,\infty), X)\), and (b) all approximation results for strongly continuous semigroups extend to bi-continuous ones (The shift semigroup is not strongly continuous in \(C_0([0,\infty), X)\) with respect to the norm topology but only with respect to the topology of uniform convergence on compact subsets of \([0,\infty)\). For a discussion and further references on “bi-continuous semigroups,” see [8]). Finally, the implication (III) \(\implies\) (I) is due to the observation that the shift semigroup \(T(t)f = f(t+\cdot)\) on \(C_0([0,\infty), X)\) satisfies (a) \(T(t)f(0) = f(t)\)
for \( t \geq 0 \) and (b) \( R(\lambda, A)f(0) = \int_0^\infty e^{-\lambda t} f(t) \, dt = \int_0^\infty e^{-\lambda t} f(t) \, dt = \hat{f}(\lambda) \) for \( \text{Re}(\lambda) > 0 \).

\[
\begin{align*}
\text{Corollary 1.} & \quad \text{Let } P, Q \text{ be given by (1) and let } r(z) = \frac{P(z)}{Q(z)} = \frac{b_1}{\lambda_1 - z} + \frac{b_2}{\lambda_2 - z} + \ldots + \frac{b_q}{\lambda_q - z} \\
& \quad \text{be the subdiagonal Padé approximation scheme of the exponential of order } m = 2q - 1, \text{ where } \lambda_i (1 \leq i \leq q) \text{ are the } q \text{ distinct roots of the polynomial } Q \text{ and } \\
& \quad b_i := \frac{P(\lambda_i)}{\prod_{j=1, j \neq i}^q (\lambda_j - \lambda_i)}.
\end{align*}
\]

Let \( X \) be a Banach space, \( f \in C_b([0, \infty), X) \) with Laplace transform \( \hat{f}(\lambda) = \int_0^\infty e^{-\lambda t} f(t) \, dt \) for \( \text{Re}(\lambda) > 0 \). If \( f \) is \((m+1)\)-times continuously differentiable with \( f^{(m+1)} \in C_b([0, \infty), X) \), then

\[
\left\| \sum_{j=1}^q \frac{b_j}{t} \hat{f}\left(\frac{\lambda_j}{t}\right) - f(t) \right\| \leq C_r t^{m+1} \| f^{(m+1)} \|_\infty,
\]

where the constants \( C_r \) are as in Theorem 3.1.

4. Rational best approximations. We shall now point to an alternative way to approximate semigroups via rational approximations \( r(z) = \frac{P(z)}{Q(z)} \) of the exponential function. To our knowledge, the following ‘rational best-approximations’ approach \([13]\) to the exponential function is a new concept. Here is the main idea. We observe first that

\[
e^{tz} = \int_0^\infty e^{zs} \, dH(t), \quad \text{Re}(z) \leq 0, \quad t \geq 0,
\]

where \( H(t) \) is the Heaviside function (i.e., \( H(t) = 0 \) if \( 0 \leq s \leq t \) and \( H(t) = 1 \) if \( s > t \)). Now, let \( z \to r(z) = \frac{P(z)}{Q(z)} \) be a rational function with \( 1 + \text{deg}(P) = \text{deg}(Q) = q, r(0) = 1 \) and whose poles \( b_i \) are all simple with \( \text{Re}(b_i) > 0 \) \((1 \leq i \leq q)\). Then

\[
r(z) = \frac{B_1}{b_1 - z} + \frac{B_2}{b_2 - z} + \ldots + \frac{B_q}{b_q - z}
\]

with

\[
B_i := \frac{P(b_i)}{\prod_{j=1, j \neq i}^q (b_j - b_i)}.
\]

Let \( B \in \mathbb{C} \) and \( \text{Re}(b) > 0 \). Then

\[
\frac{B}{b - z} = \int_0^\infty e^{zs} \, d\alpha_{b, B}(s), \quad \text{Re}(z) \leq 0,
\]

where \( \alpha_{b, B}(s) := \frac{B}{b} [1 - e^{-bs}] \). In particular,

\[
r(z) = \frac{B_1}{b_1 - z} + \frac{B_2}{b_2 - z} + \ldots + \frac{B_q}{b_q - z} = \int_0^\infty e^{zs} \, d\alpha_r(s) \quad (\text{Re}(z) \leq 0),
\]

where \( \alpha_r(s) = \alpha_{b_1, B_1}(s) + \alpha_{b_2, B_2}(s) + \ldots + \alpha_{b_q, B_q}(s) \), and for \( \text{Re}(z) \leq 0 \) and \( t \geq 0 \),

\[
r(z) - e^{tz} = \int_0^\infty e^{zs} \, d[\alpha_r(s) - H(t)] = \int_0^\infty ze^{zs} [\alpha_r(s) - H(t)] \, ds.
\]
since \( \alpha_r(0) - H_t(0) = 0 \), and
\[
\alpha_r(\infty) - H_t(\infty) = \sum_{i=1}^{q} \frac{B_i}{b_i} - 1 = r(0) - 1 = 0.
\]
In particular,
\[
|r(z) - e^{tz}| \leq |z|\|\alpha_r - H_t\|_1.
\]
Thus, we call a rational function of the form (10) with \( r(0) = 1 \) and \( \text{Re}(b_i) > 0 \) a rational best approximation of degree \((q-1, q)\) of the exponential function at \( t \geq 0 \) if \( \|\alpha_r - H_t\|_1 \) is minimal, where
\[
\alpha_r(s) := \frac{B_1}{b_1}[1 - e^{-b_1s}] + \frac{B_2}{b_2}[1 - e^{-b_2s}] + \ldots + \frac{B_q}{b_q}[1 - e^{-b_qs}]
\]
\[
= 1 - \frac{B_1}{b_1}e^{-b_1s} - \frac{B_2}{b_2}e^{-b_2s} - \ldots - \frac{B_q}{b_q}e^{-b_qs} \quad (s \geq 0).
\]
As a first example, we compute the rational best approximation of degree \((0, 1)\) of the exponential function \( t \to e^{tz} \) (\( \text{Re}(z) \leq 0 \)) at a given value \( t > 0 \). That is, we find \( r(z) = \frac{p(z)}{q(z)} \) with \( r(0) = 1 \) (or \( B = b \)) such that \( \|\alpha_{(0,1)} - H_t\|_1 \) is minimal, where
\[
\alpha_{(0,1)}(s) = \frac{B}{b}[1 - e^{-bs}] = 1 - e^{-bs}.
\]
Now,
\[
\|\alpha_{(0,1)} - H_t\|_1 = \int_0^t |\alpha_{(0,1)}(s)| \, ds + \int_t^\infty |\alpha_{(0,1)}(s) - 1| \, ds = t + 2b e^{-bt} - 1
\]
has a minimum when \((1 + bt)e^{-bt} = 1/2\) or when \( b = 1.67835/t \) (MATLAB). In this case,
\[
\|\alpha_{(0,1)} - H_t\|_1 = 0.6266t. \tag{11}
\]
In particular, if \( r_t(z) = \frac{1.67835}{1.67835 - tz} \), then \( |r_t(z) - e^{tz}| \leq 0.6266t \, |z| \) for \( \text{Re}(z) \leq 0 \).

Similarly, the rational best approximation
\[
r(z) = \frac{a + bz}{a - z} = -b + \frac{a(b+1)}{a - z}
\] of degree \((1, 1)\) of the exponential at \( t \geq 0 \) can be determined. Let \( a, b > 0 \) and \( \text{Re}(z) \leq 0 \). Then
\[
|r(z) - e^{tz}| = \left| - \int_0^\infty z e^{sz} \left[ 1 - (1 + b)e^{-as} - H_t(s) \right] \, ds \right|
\]
\[
\leq |z| \left[ \int_0^t |1 - (1 + b)e^{-as}| \, ds + \int_t^\infty |(1 + b)e^{-as}| \, ds \right]
\]
\[
= |z| \left[ t - \frac{2}{a} - \frac{2}{2} \ln(1 + b) + \frac{1 + b}{a} + \frac{2(1 + b)}{a} e^{-at} \right]
\]
\[
= |z| \cdot \|\alpha_{(1,1)} - H_t\|_1,
\]
where \( \alpha_{(1,1)}(s) := 1 - (1 + b)e^{-as} \). Using MATLAB we obtain that
\[
\|\alpha_{(1,1)} - H_t\|_1 = 0.545816 \cdot t. \tag{13}
\]
if \( a = \frac{1.91795}{t} \) and \( b = 0.545816 \). In particular, if
\[
r_t(z) = \frac{1.91795 + 0.545816 \cdot t \cdot z}{1.91795 - tz} = -0.545816 + \frac{2.9648 \cdot \frac{1}{t}}{1.91795 - z},
\]
In this case, then computation shows that the estimate (11) can not be improved if $b_1$ and $b_2$ are real. Thus, we consider
\[ r(z) = \frac{B_1}{b_1 - z} + \frac{B_2}{b_2 - z} \quad (\text{Re}(z) \leq 0) \]
of degree $(1, 2)$ with $r(0) = \frac{B_1}{b_1} + \frac{B_2}{b_2} = 1$. We remark first that a simple, yet tedious computation shows that the estimate (11) can not be improved if $b_1$ and $b_2$ are real.

Let \((12) - (16)\) and Proposition 1 one obtains the following approximation results.

In particular, if
\[ r_t(z) = \frac{2.93445 - 1.57046i}{1.9833 + 1.619i - tz} + \frac{2.93445 + 1.57046i}{1.9833 - 1.619i - tz} \quad (16) \]
then \(|r_t(z) - e^{tz}| \leq 0.3533t \cdot |z|\) for all $t \geq 0$ and $\text{Re}(z) \leq 0$.

As immediate consequence of the Hille-Phillips functional calculus in combination with \((12) - (16)\) and Proposition 1 one obtains the following approximation results.

**Proposition 2.** Let \((A, D(A))\) be the generator of a bi-continuous semigroup \(T(t)\) on a Banach space \(X\) with \(\|T(t)\| \leq M\) for all $t \geq 0$. Then, for all $t > 0$ and $x \in D(A)$,
\begin{aligned}
&\left\| \frac{1.67835}{t} R \left( \frac{1.67835}{t}, A \right) x - T(t)x \right\| \leq 0.6266 M \cdot t \|Ax\|, \\
&\left\| -0.545816x + \frac{2.9648}{t} R \left( \frac{1.67835}{t}, A \right) x - T(t)x \right\| \leq 0.545816 M \cdot t \|Ax\|, \\
&\left\| B \frac{t}{7} \tilde{f} \left( \frac{1.67835}{t} \right) + B \frac{t}{7} \tilde{f} \left( \frac{b}{t} \right) - f(t) \right\| \leq 0.3533 M \cdot t \|Ax\|,
\end{aligned}

where $B = 2.93445 - 1.57046i$ and $b = 1.9833 + 1.619i$.

**Corollary 2.** Let $X$ be a Banach space, $f \in C_b([0, \infty), X)$ with Laplace transform $\tilde{f}(\lambda) = \int_0^\infty e^{-\lambda t} f(t) dt$ for $\text{Re}(\lambda) > 0$. If $f$ is continuously differentiable with $f' \in C_b([0, \infty), X)$, then

\begin{aligned}
&(i)\quad \left\| \frac{1.67835}{t} \tilde{f} \left( \frac{1.67835}{t} \right) - f(t) \right\| \leq 0.6266 \cdot t \|f'\|_\infty, \\
&(ii)\quad \left\| -0.545816x + \frac{2.9648}{t} \tilde{f} \left( \frac{1.67835}{t} \right) - f(t) \right\| \leq 0.545816 \cdot t \|f'\|_\infty, \\
&(iii)\quad \left\| B \frac{t}{7} \tilde{f} \left( \frac{1.67835}{t} \right) + B \frac{t}{7} \tilde{f} \left( \frac{b}{t} \right) - f(t) \right\| \leq 0.3533 \cdot t \|f'\|_\infty,
\end{aligned}

where $B = 2.93445 - 1.57046i$ and $b = 1.9833 + 1.619i$.

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E-mail address: neubrand@math.lsu.edu
E-mail address: kozer@rwu.edu
E-mail address: tesa@fa.uni-tuebingen.de