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Error Bounds for Padé Approximations of e^{-z} on the Imaginary Axis

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I. INTRODUCTION

This paper is concerned with the approximation of e^{-z} by its Padé approximants. Error bounds are obtained for $z = j\omega$, where j is the purely imaginary unit and $\omega \in \mathbb{R}$. By employing a similar method of Braess [1], it can be shown that, for m and n belonging to $\mathbb{N}_0 = \{0, 1, 2, ...\}$ such that $m + 2 \geqslant n$,

$$|e^{-j\omega} - R_{mn}(j\omega)| \leqslant \frac{n!\,m!}{(n+m)!\,(n+m+1)!}\,\omega^{n+m+1}, \qquad \omega \geqslant 0,$$

where $R_{mn}(z)$ is the (m,n)-Padé approximant of e^{-z}. The results presented are related to those of Braess [1]; of Newman [3], which concern with approximation on the interval $[-1, 1]$, and of Trefethen [5] on a disk. The results here contrast to theirs by considering approximation properties along the imaginary axis, and by deriving tight error bounds which are not asymptotic in nature. Moreover, only elementary mathematical induction technique is involved.

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II. MAIN RESULTS

We start by considering the (m, n)-Padé approximant of e^{-z}, where $m, n \in \mathbb{N}_0$, given by Perron [2] (see also Braess [1] and Petrushev and Popov [4, p. 96])

$$R_{mn}(z) = \frac{p_{mn}(z)}{q_{mn}(z)},$$

where

$$p_{mn}(z) = \int_0^\infty t^n (t-z)^m e^{-t}\, dt \tag{1}$$

$$q_{mn}(z) = \int_0^\infty t^m (t+z)^n e^{-t}\, dt. \tag{2}$$

Here $R_{mn}(z)$ is a rational function with numerator and denominator degree equal to m and n, respectively. Then, we have the following proposition.

PROPOSITION 1. *For $m, n \in \mathbb{N}_0$ and $\omega \geqslant 0$,*

$$|e^{-j\omega} q_{nm}(j\omega) - p_{mn}(j\omega)| \leqslant \frac{n!\,m!}{(n+m+1)!}\, \omega^{n+m+1}.$$

Proof. Since

$$\begin{aligned} &e^{-z} q_{mn}(z) - p_{mn}(z) \\ &\quad = \int_0^\infty t^m (t+z)^n e^{-(t+z)}\, dt - \int_0^\infty t^n (t-z)^m e^{-t}\, dt \\ &\quad = -\int_{-z}^0 (t+z)^n t^m e^{-(t+z)}\, dt \\ &\quad = (-z)^{n+m+1} \int_0^1 (u-1)^n u^m e^{(u-1)z}\, du \\ &\quad = (-1)^{m+1} z^{n+m+1} \int_0^1 (1-u)^n u^m e^{(u-1)z}\, du, \end{aligned}$$

then

$$\begin{aligned}
|e^{-z}q_{mn}(z)-p_{mn}(z)| &= |z|^{n+m+1}\left|\int_0^1 (1-u)^n u^m e^{(u-1)z}\,du\right| \\
&= |z|^{n+m+1}\left|\int_0^1 u^n(1-u)^m e^{-uz}\,du\right| \\
&\leqslant |z|^{n+m+1}\int_0^1 u^n(1-u)^m\,|e^{-uz}|\,du \\
&\leqslant |z|^{n+m+1}\max_{0\leqslant u\leqslant 1}|e^{-uz}|\int_0^1 u^n(1-u)^m\,du \\
&= |z|^{n+m+1}\max_{0\leqslant u\leqslant 1}|e^{-uz}|\frac{n!\,m!}{(n+m+1)!}.
\end{aligned}$$

For $z=j\omega$, $\omega\geqslant 0$, we have

$$\max_{0\leqslant u\leqslant 1}|e^{-uz}|=\max_{0\leqslant u\leqslant 1}|e^{-ju\omega}|=1$$

and hence the result follows. ▮

The upper bound in Proposition 1 is tight since it corresponds to exactly the first non-zero error term (see also Petrushev and Popov [4, pp. 96–98]).

Now our objective is to find a lower bound for $|q_{mn}(j\omega)|$. In order to achieve this goal, we need a recurrence formula for the expression of $|q_{mn}(j\omega)|^2$ which is given in the following lemma.

LEMMA 2. *Let*

$$K_{m,n}(\omega) := |q_{mn}(j\omega)|^2 \equiv \left|\int_0^\infty t^m(t+j\omega)^n e^{-t}\,dt\right|^2,$$

then

$$\begin{aligned}
K_{m,n+1}(\omega) &= K_{m+1,n}(\omega)+\omega^2 K_{m,n}(\omega) \\
&\quad -\omega^2 n(2m+n+1)K_{m,n-1}(\omega) \\
&\quad -\omega^2 n(n-1)K_{m+1,n-2}(\omega)+\omega^4 n(n-1)K_{m,n-2}(\omega). \qquad (3)
\end{aligned}$$

Proof. Let $q_{m,n}(z)\equiv q_{mn}(z)$; then

$$\begin{aligned}
q_{m,n}(j\omega) &:= \int_0^\infty t^m(t+j\omega)^n e^{-t}dt \\
&= \int_0^\infty t^{m+1}(t+j\omega)^{n-1}e^{-t}\,dt + j\omega\int_0^\infty t^m(t+j\omega)^{n-1}e^{-t}\,dt \\
&= q_{m+1,n-1}(j\omega)+j\omega q_{m,n-1}(j\omega). \qquad (4)
\end{aligned}$$

Also

$$q_{m,n}(j\omega) = \int_0^\infty t^m (t+j\omega)^n e^{-t}\,dt$$
$$= [-t^m (t+j\omega)^n e^{-t}]_0^\infty + \int_0^\infty e^{-t} d[t^m (t+j\omega)^n]$$
$$= \int_0^\infty [m t^{m-1}(t+j\omega)^n + n t^m (t+j\omega)^{n-1}] e^{-t}\,dt$$
$$= m q_{m-1,n}(j\omega) + n q_{m,n-1}(j\omega). \tag{5}$$

Now, by the definition of $K_{m,n}(\omega)$, we have

$$\begin{aligned} K_{m,n}(\omega) &= q_{m,n}(j\omega) q_{m,n}(-j\omega) \\ &= (q_{m+1,n-1}(j\omega) + j\omega q_{m,n-1}(j\omega)) \\ &\quad \times (q_{m+1,n-1}(-j\omega) - j\omega q_{m,n-1}(-j\omega)) \\ &= K_{m+1,n-1}(\omega) + \omega^2 K_{m,n-1}(\omega) + j\omega L_{m,n-1}(j\omega) \end{aligned} \tag{6}$$

after expansion and with

$$L_{m,n}(j\omega) := q_{m,n}(j\omega) q_{m+1,n}(-j\omega) - q_{m+1,n}(j\omega) q_{m,n}(-j\omega).$$

From (4) and (5), we have

$$\begin{aligned} &q_{m,n}(j\omega) q_{m+1,n}(-j\omega) \\ &\quad = (q_{m+1,n-1}(j\omega) + j\omega q_{m,n-1}(j\omega))[(m+1) q_{m,n}(-j\omega) \\ &\qquad + n q_{m+1,n-1}(-j\omega)] \\ &\quad = (q_{m+1,n-1}(j\omega) + j\omega q_{m,n-1}(j\omega))[(m+1)(q_{m+1,n-1}(-j\omega) \\ &\qquad - j\omega q_{m,n-1}(-j\omega)) + n q_{m+1,n-1}(-j\omega)] \\ &\quad = (q_{m+1,n-1}(j\omega) + j\omega q_{m,n-1}(j\omega))[(m+n+1) q_{m+1,n-1}(-j\omega) \\ &\qquad - j\omega(m+1) q_{m,n-1}(-j\omega)] \\ &\quad = (m+n+1) K_{m+1,n-1}(\omega) + (m+1)\omega^2 K_{m,n-1}(\omega) \\ &\qquad + j\omega[(m+n+1) q_{m,n-1}(j\omega) q_{m+1,n-1}(-j\omega) \\ &\qquad - (m+1) q_{m+1,n-1}(j\omega) q_{m,n-1}(-j\omega)]. \end{aligned} \tag{7}$$

Taking the conjugate of (7) we obtain

$$\begin{aligned}
&q_{m,n}(-j\omega)q_{m+1,n}(j\omega)\\
&\quad=(m+n+1)K_{m+1,n-1}(\omega)+(m+1)\omega^2K_{m,n-1}(\omega)\\
&\qquad-j\omega[(m+n+1)q_{m,n-1}(-j\omega)q_{m+1,n-1}(j\omega)\\
&\qquad-(m+1)q_{m+1,n-1}(-j\omega)q_{m,n-1}(j\omega)]. \qquad (8)
\end{aligned}$$

Subtracting (8) from (7) and by the definition of $L_{m,n}(j\omega)$, we have

$$\begin{aligned}
L_{m,n}(j\omega)&=q_{m,n}(j\omega)q_{m+1,n}(-j\omega)-q_{m+1,n}(j\omega)q_{m,n}(-j\omega)\\
&=j\omega[nq_{m,n-1}(j\omega)q_{m+1,n-1}(-j\omega)+nq_{m+1,n-1}(j\omega)q_{m,n-1}(-j\omega)\\
&=j\omega nP_{m,n-1}(j\omega), \qquad (9)
\end{aligned}$$

where

$$P_{m,n}(j\omega):=q_{m,n}(j\omega)q_{m+1,n}(-j\omega)+q_{m+1,n}(j\omega)q_{m,n}(-j\omega).$$

By adding (7) and (8), we have

$$\begin{aligned}
P_{m,n}(j\omega)&=q_{m,n}(j\omega)q_{m+1,n}(-j\omega)+q_{m+1,n}(j\omega)q_{m,n}(-j\omega)\\
&=2(m+n+1)K_{m+1,n-1}(\omega)+2(m+1)\omega^2K_{m,n-1}(\omega)\\
&\quad+j\omega(2m+n+2)[q_{m,n-1}(j\omega)q_{m+1,n-1}(-j\omega)\\
&\quad-q_{m+1,n-1}(j\omega)q_{m,n-1}(-j\omega)]\\
&=2(m+n+1)K_{m+1,n-1}(\omega)+2(m+1)\omega^2K_{m,n-1}(\omega)\\
&\quad+j\omega(2m+n+2)L_{m,n-1}(j\omega). \qquad (10)
\end{aligned}$$

From (6), (9), and (10), we obtain

$$\begin{aligned}
K_{m,n+1}(\omega)&=K_{m+1,n}(\omega)+\omega^2K_{m,n}(\omega)+j\omega L_{m,n}(j\omega)\\
&=K_{m+1,n}(\omega)+\omega^2K_{m,n}(\omega)-\omega^2nP_{m,n-1}(j\omega)\\
&=K_{m+1,n}(\omega)+\omega^2K_{m,n}(\omega)-2\omega^2n(m+n)K_{m+1,n-2}(\omega)\\
&\quad-2\omega^4n(m+1)K_{m,n-2}(\omega)-j\omega^3n(2m+n+1)L_{m,n-2}(j\omega)\\
&=K_{m+1,n}(\omega)+\omega^2K_{m,n}(\omega)-2\omega^2n(m+n)K_{m+1,n-2}(\omega)\\
&\quad-2\omega^4n(m+1)K_{m,n-2}(\omega)-\omega^2n(2m+n+1)[K_{m,n-1}(\omega)\\
&\quad-K_{m+1,n-2}(\omega)-\omega^2K_{m,n-2}(\omega)]\\
&=K_{m+1,n}(\omega)+\omega^2K_{m,n}(\omega)-\omega^2n(2m+n+1)K_{m,n-1}(\omega)\\
&\quad-\omega^2n(n-1)K_{m+1,n-2}(\omega)+\omega^4n(n-1)K_{m,n-2}(\omega)
\end{aligned}$$

after simplification. ∎

From the recurrence formula in Lemma 2, we obtain the following proposition regarding the modulus of $q_{mn}(j\omega)$:

PROPOSITION 3. *For $m, n \in \mathbb{N}_0$, $|q_{mn}(j\omega)|^2 \equiv K_{m,n}(\omega)$ is given by*

$$K_{m,n}(\omega) = \begin{cases} (m!)^2 \left[\sum_{r=0}^{n-1} \binom{n}{r} \prod_{i=1}^{n-r} (m-r+i)(m+i)\omega^{2r} + \omega^{2n} \right] & \text{for } n \geq 1 \\ (m!)^2 & \text{for } n = 0. \end{cases} \tag{11}$$

Proof. We use proof by mathematical induction on n. For $n=0$ and $m \in \mathbb{N}_0$, we have the LHS of (11) as

$$|q_{mn}(j\omega)|^2 = \left| \int_0^{\infty} t^m e^{-t}\, dt \right|^2 = (m!)^2.$$

while the RHS of (11) gives also $(m!)^2$. Similarly, for $n=1$, $K_{m,1}(\omega) = (m!)^2 [(m+1)^2 + \omega^2]$ and for $n=2$, $K_{m,2}(\omega) = (m!)^2 [(m+1)^2 (m+2)^2 + 2m(m+1)\omega^2 + \omega^4]$. It is easy to verify that (11) gives the same expressions.

Assume that the proposition is true for $n = h$, $h-1$, $h-2$, where $h \in \mathbb{N}_0$, $h \geq 2$, and $m \in \mathbb{N}_0$. Then from Lemma 2, we have

$$\begin{aligned} K_{m,h+1} = {} & K_{m+1,h} + \omega^2 K_{m,h} - \omega^2 h(2m+h+1) K_{m,h-1} \\ & - \omega^2 h(h-1) K_{m+1,h-2} + \omega^4 h(h-1) K_{m,h-2}, \end{aligned} \tag{12}$$

where we have dropped the argument ω for clarity. Now, we examine the coefficients of ω^{2r} $(r = 0, 1, ..., h+1)$ in $K_{m,h+1}$ by considering (12).

The constant term $(r=0)$ is equal to that of $K_{m+1,h}$ (from (12)) which is $[(m+1+h)!]^2$. This is given by the proposition with $n = h+1$. The coefficient of ω^2 on the RHS of (12) is given by

$$\begin{aligned} & [(m+1)!]^2 h \prod_{i=1}^{h-1} (m+i)(m+1+i) + [(m+h)!]^2 \\ & \quad - h(2m+h+1)[(m+h-1)!]^2 - h(h-1)[(m+h-1)!]^2 \\ & = [(m+h-1)!]^2 \, [h(m+1)(m+h) \\ & \quad + (m+h)^2 - h(2m+h+1) - h(h-1)] \\ & = [(m+h-1)!]^2 \, (h+1)m(m+h) \\ & = (m!)^2 \, (h+1) \prod_{i=1}^{h} (m-1+i)(m+i) \end{aligned}$$

which is the coefficient of ω^2 in (11) when $n = h+1$.

For ω^{2r}, where $2 \leqslant r \leqslant h-1$, the coefficient is obtained from (12) as

$$[(m+1)!]^2 \binom{h}{r} \prod_{i=1}^{h-r} (m+1-r+i)(m+1+i)$$
$$+(m!)^2 \binom{h}{r-1} \prod_{i=1}^{h-r+1} (m-r+1+i)(m+i)$$
$$-h(2m+h+1)(m!)^2 \binom{h-1}{r-1} \prod_{i=1}^{h-r} (m-r+1+i)(m+i)$$
$$-h(h-1)[(m+1)!]^2 \binom{h-2}{r-1} \prod_{i=1}^{h-r-1} (m+2-r+i)(m+1+i)$$
$$+h(h-1)(m!)^2 \binom{h-2}{r-2} \prod_{i=1}^{h-r} (m-r+2+i)(m+i)$$
$$=(m!)^2 \prod_{i=1}^{h-r} (m+1-r+i)(m+i) \left\{(m+1)(m+1+h-r)\binom{h}{r}\right.$$
$$\left.+(m-h)(m+1+h-r)\binom{h}{r-1}\right\}$$
$$=(m!)^2 \binom{h+1}{r} \prod_{i=1}^{h+1-r} (m-r+i)(m+i)$$

which is the coefficient of ω^{2r} for $2 \leqslant r \leqslant h-1$ in (11) with $n=h+1$.

Now, consider the coefficient of ω^{2h}. From (12) we obtained the coefficient as

$$[(m+1)!]^2 + (m!)^2 h(m-h+2)(m+1)$$
$$-h(2m+h+1)(m!)^2 + h(h-1)(m!)^2$$
$$=(m!)^2\,(h+1)(m-h+1)(m+1)$$

which is the coefficient of ω^{2h} in (11) when $n=h+1$.

Finally, the coefficient of ω^{2h+2} in (12) is $(m!)^2$ which is also that of ω^{2h+2} in (11) with $n=h+1$.

Hence, we have shown that the expression in (11) is also true for $n=h+1$ if the cases $n=h$, $h-1$, $h-2$ are true with $m \in \mathbb{N}_0$. By the principle of mathematical induction, we can conclude that (11) is true for all $m, n \in \mathbb{N}_0$. ∎

The following result gives a lower bound for $|q_{mn}(j\omega)|$ as a corollary of Proposition 3.

COROLLARY 4. *For $m, n \in \mathbb{N}_0$ such that $m+2 \geqslant n$ and $\omega \geqslant 0$,*

$$|q_{mn}(j\omega)| \geqslant |q_{mn}(0)| = (m+n)!.$$

Proof. From (11), the coefficient of ω^{2r}, where $r < n$, is given by

$$(m!)^2 \binom{n}{r} \prod_{i=1}^{n-r} (m-r+i)(m+i)$$

which is non-negative as long as $(m-r+1) \geqslant 0$. This requires that $m-n+2 \geqslant 0$ for all coefficients in $|q_{mn}(j\omega)|^2$ to be non-negative. Hence,

$$|q_{mn}(j\omega)|^2 = K_{m,n}(\omega) \geqslant K_{m,n}(0) = [(m+n)!]^2 = |q_{mn}(0)|^2. \quad \blacksquare$$

It is well known that for $m+2 \geqslant n$, the denominator $q_{mn}(z)$ is analytic in the open RHP (see Saff and Varga [6], for example). In fact, from Corollary 4, we can see that $m+2 \geqslant n$ gives all coefficients in $q_{mn}(j\omega)$ non-negative for this class of Padé approximants. Now, we can state the main result as follows.

THEOREM 5. *For $m, n \in \mathbb{N}_0$ such that $m+2 \geqslant n$ and $\omega \geqslant 0$,*

$$\left| e^{-j\omega} - \frac{p_{mn}(j\omega)}{q_{mn}(j\omega)} \right| \leqslant \frac{n!\,m!}{(n+m)!\,(n+m+1)!} \omega^{n+m+1}. \tag{13}$$

Proof. From Proposition 1, we have for $m, n \in \mathbb{N}_0$ and $\omega \geqslant 0$

$$|e^{-j\omega} q_{mn}(j\omega) - p_{mn}(j\omega)| \leqslant \frac{n!\,m!}{(n+m+1)!} \omega^{n+m+1}.$$

Also, Corollary 4 gives

$$\frac{1}{|q_{mn}(j\omega)|} \leqslant \frac{1}{(m+n)!}$$

when $m+2 \geqslant n$. Hence, the result follows. $\blacksquare$

The result in Theorem 5 is tight from the derivation shown with equality holding when $\omega = 0$. The upper bound in Theorem 5 corresponds to exactly the first non-zero coefficient of the error in terms of its Maclaurin series expansion. For example, with $m = 2$ and $n = 3$, we have

$$\left| e^{-j\omega} - \frac{p_{23}(j\omega)}{q_{23}(j\omega)} \right| = \frac{1}{7200} \omega^6 - \frac{37}{5880000} \omega^8 + \frac{47153}{518616000000} \omega^{10} - \cdots,$$

while the RHS of (13) gives

$$\frac{3!2!}{(3+2)!(3+2+1)!}\omega^{3+2+1}=\frac{1}{7200}\omega^6.$$

In passing, it is remarked that when $n-2 \leqslant m \leqslant n$,

$$\left| e^{-j\omega} - \frac{p_{mn}(j\omega)}{q_{mn}(j\omega)} \right| \leqslant 2 \tag{14}$$

which results from the A-acceptability of Padé approximations to e^z, since

$$\left| \frac{p_{mn}(j\omega)}{q_{mn}(j\omega)} \right| \leqslant 1$$

(see Wanner *et al.* [7]). In this case, it is obvious that the bound in (13) is weak for large ω. Indeed, this is generally true for all cases when ω is large since the LHS of (13) is at most of order ω^{m-n}. Based on the observation in (14), we state the following proposition as a consequence.

PROPOSITION 6. *For $m, n \in \mathbb{N}_0$ such that $n-2 \leqslant m \leqslant n$ and $\omega \geqslant 0$,*

$$\left| e^{-j\omega} - \frac{p_{mn}(j\omega)}{q_{mn}(j\omega)} \right| \leqslant \min\left(2, \frac{n!m!}{(n+m)!(n+m+1)!}\omega^{n+m+1}\right). \quad \blacksquare$$

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