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THE BEHAVIOR OF THE PADÉ TABLE FOR THE EXPONENTIAL

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In this paper we survey recent results and present some new theorems on the behavior of Padé approximants for e^{-z}. The new results include necessary and sufficient conditions for (1) a sequence of approximants to be pole-free in an infinite sector, and (2) a sequence of approximants to converge geometrically in the uniform norm over an infinite sector.

1 Introduction

While the study of the Padé table for the exponential function dates back to Padé's thesis, there has been renewed interest in the subject because of its usefulness in certain numerical schemes for solving parabolic differential equations. Several recent papers have appeared which consider the questions of location of zeros and poles, regions of convergence, and degree of convergence of sequences from the table (see [3], [9], [10], [14], [16]). The purpose of the present paper is to survey some of these results and also to establish some new theorems. In this first section we introduce the necessary notation, in Sec. 2 we discuss zero and pole-free regions, and in Sec. 3 we consider the degree of convergence of Padé approximants in unbounded regions.

To be specific we shall deal with the complex negative exponential function e^{-z}. For each pair (ν,n) of nonnegative integers the <u>Padé approximant</u> $R_{\nu,n}(z)$ <u>of type</u> (ν,n) for e^{-z} is defined as that unique rational function with numerator degree ν, denominator degree n, which has greatest contact with e^{-z} at the origin, i.e.,

$$(1.1)\quad e^{-z} - R_{\nu,n}(z) = O(z^{n+\nu+1}) \quad \text{as} \quad z\to 0 \quad .$$

Explicitly it is known [6] that $R_{\nu,n}(z) = Q_{\nu,n}(z)/P_{\nu,n}(z)$, where

$$(1.2)\quad Q_{\nu,n}(z) = \sum_{j=o}^{\nu} \frac{(n+\nu-j)!\nu!(-z)^j}{(n+\nu)!j!(\nu-j)!} \quad ,$$

and

$$(1.3)\quad P_{\nu,n}(z) = \sum_{j=o}^{n} \frac{(n+\nu-j)!n!z^j}{(n+\nu)!j!(n-j)!} \quad .$$

The polynomials $Q_{\nu,n}(z)$ and $P_{\nu,n}(z)$ are referred to respectively as the <u>Padé numerator</u> and <u>Padé denominator</u> of type (ν,n) for e^{-z} . From the representations (1.2) and (1.3) it is apparent that $Q_{\nu,n}(z) = P_{n,\nu}(-z)$, and so any result on the location of the poles of Padé approximants to e^{-z} has a reformulation in terms of zeros.

The Padé approximants $R_{\nu,n}(z)$ are usually studied in the context of the following doubly infinite array known as the <u>Padé table</u>:

$$(1.4)\quad \begin{bmatrix} R_{0,0} & R_{1,0} & R_{2,0} & \cdots \\ R_{0,1} & R_{1,1} & R_{2,1} & \cdots \\ R_{0,2} & R_{1,2} & R_{2,2} & \cdots \\ \vdots & \vdots & \vdots & \end{bmatrix} \quad .$$

Notice that the first row of the table consists of the partial sums $R_{\nu,o}(z) = \sum_{k=o}^{\nu} (-z)^k/k!$ of e^{-z} and that the first column is composed of the reciprocals of the partial sums for the positive exponential, i.e., $R_{o,n}(z) = [\sum_{k=o}^{n} z^k/k!]^{-1}$.

2 Unbounded pole-free regions

The asymptotic behavior of the poles of the first column of (1.4), i.e., the zeros of the partial sums $s_n(z) = \sum_{k=o}^{n} z^k/k!$, was studied by Szegö [13] and Dieudonné [2]. As a consequence of their results it follows that any infinite sector with vertex at the origin contains infinitely many poles of the sequence $\{R_{o,n}(z)\}_{n=o}^{\infty}$. By way of contrast it is shown in R.S. Varga's thesis [17] that the infinite half-strip $|y| \leq \sqrt{6}$, $x \geq 0$, is free of poles of the whole sequence $\{R_{o,n}(z)\}_{n=o}^{\infty}$. More recently, Newman and Rivlin ([4], [5]) established that there exists an unbounded parabolic region, namely

(2.1) $y^2 \leq dx \quad , \quad x \geq 0 \quad , \; d \doteq 0.745 \quad ,$

which is pole-free for the sequence $\{R_{o,n}(z)\}_{n=o}^{\infty}$. Furthermore they proved that for this sequence parabolic growth characterizes the largest pole-free region symmetric about the positive real axis.

Using continued fraction techniques the authors were able to improve upon the result of (2.1) and also to obtain similar results for all the columns of the table (1.4). In stating this theorem it is convenient to introduce the normalized Padé approximants $R_{\nu,n}((\nu+1)z)$.

THEOREM 2.1. (Saff, Varga [8], [11]). For all $\nu \geq 0$, $n \geq 0$, the normalized Padé approximant $R_{\nu,n}((\nu+1)z)$ has no poles in the unbounded parabolic region

(2.2) $P_1 := \{z = x + iy : y^2 \leq 4(x+1) \quad , \; x > -1\}$.

Moreover, every boundary point of P_1 is a limit point of poles of the collection $\{R_{\nu,n}((\nu+1)z)\}_{\nu=o,n=o}^{\infty\;,\;\infty}$.

In particular, Theorem 2.1 implies that the first column of the table (1.4), for which $\nu=0$, is pole-free in P_1 (a region larger than that of (2.1)) and, in general, the $(\nu+1)$st column $\{R_{\nu,n}(z)\}_{n=0}^{\infty}$ is pole-free in the parabolic region

(2.3) $$P_{\nu+1} := \{z=x+iy : y^2 \leq 4(\nu+1)(x+\nu+1) \,,\ x > -(\nu+1)\} \,.$$

These facts have proved useful in approximation estimates for the matrix exponential as discussed in a recent paper of Van Loan [15].

While Theorem 2.1 is sharp, it does not include the fact that for an arbitrary _fixed_ ν the largest pole-free region for the sequence $\{R_{\nu,n}(z)\}_{n=0}^{\infty}$ has parabolic growth. We shall prove this in

THEOREM 2.2. _For each fixed_ $\nu \geq 0$, _the Padé approximant_ $R_{\nu,n}(z)$ _for_ e^{-z} _has a pole of the form_

(2.4) $$(n+\sqrt{n}\, x_{\nu,n}) + i\sqrt{n}\, y_{\nu,n} \,, \quad \text{where} \quad x_{\nu,n} + iy_{\nu,n} \to w_\nu \,(\neq 0)$$

_as_ $n\to\infty$.

Note that as

$$\lim_{n\to\infty} \frac{ny_{\nu,n}^2}{n+\sqrt{n}\, x_{\nu,n}} = (\operatorname{Im} w_\nu)^2 \,,$$

there are poles of the $R_{\nu,n}(z)$ which asymptotically fall on the parabolic arc $y^2 = (\operatorname{Im} w_\nu)^2 x$, as $n\to\infty$. When $\nu=0$, Theorem 2.2 reduces to the known result of Newman and Rivlin [4]. The proof of Theorem 2.2 requires the following lemma:

LEMMA 2.1. _For each nonnegative integer_ ν, _the function_

(2.5) $$F_\nu(z) := \int_0^\infty t^\nu e^{-zt-t^2/2}\,dt \,, \quad (0 \leq t < \infty) \,,$$

is an entire function having at least one (finite) zero $w_\nu (\neq 0)$.

Proof. It is easy to see that $F_\nu(z)$ is entire. More precisely, on writing

$$(2.6)\quad F_\nu(z) = \sum_{k=o}^{\infty} a_k(\nu) z^k \quad ,$$

it follows from (2.5) that

$$(2.7)\quad a_k(\nu) = \frac{(-1)^k\, 2^{(\frac{k+\nu-1}{2})}\, \Gamma(\frac{k+\nu+1}{2})}{k!} \quad , \quad k \geq 0 \quad .$$

Using Stirling's formula one can verify from (2.7) that $F_\nu(z)$ is of order 2 for each ν and, moreover, $F_\nu(z)$ is an entire function of perfectly regular growth; specifically if $M_{F_\nu}(r) := \max\limits_{|z|=r} |F_\nu(z)|$, then

$$(2.8)\quad \lim_{r\to\infty} \frac{\ln M_{F_\nu}(r)}{r^2} = \frac{1}{2} \quad .$$

Now assume to the contrary that $F_\nu(z)$ has no zeros. By the Hadamard Factorization Theorem ([1,p.22]), we can express $F_\nu(z)$ as $F_\nu(z)=e^{q(z)}$, where $q(z)$ is a polynomial of degree not exceeding the order of F_ν . Hence, since F_ν is of order 2 , there exist constants α_1, α_2 such that

$$(2.9)\quad F_\nu(z) = F_\nu(0) e^{\alpha_1 z + \alpha_2 z^2} = a_o(\nu) e^{\alpha_1 z+\alpha_2 z^2} \quad , \text{ for all } z \quad .$$

Using (2.7), (2.8), and the fact that $M_{F_\nu}(r) = F_\nu(-r)$, it is easy to show that

$$\alpha_2 = \frac{1}{2} \quad , \quad \alpha_1 = -\sqrt{2}\, \Gamma(\tfrac{\nu+2}{2}) / \Gamma(\tfrac{\nu+1}{2}) \quad ,$$

and hence the right-hand member of (2.9) is completely specified. Equating the coefficients of z^2 in (2.9) results in the equation

$$\frac{2^{\frac{\nu+1}{2}}\, \Gamma(\frac{\nu+3}{2})}{2} = \frac{2^{\frac{\nu-1}{2}}\, \Gamma(\frac{\nu+1}{2})}{2} \left\{1 + \left[\frac{\sqrt{2}\, \Gamma(\frac{\nu+2}{2})}{\Gamma(\frac{\nu+1}{2})}\right]^2 \right\} ,$$

which after some minor manipulations becomes

$$(2.10)\quad \nu\left(\Gamma\left(\frac{\nu+1}{2}\right)\right)^2 = 2\left(\Gamma\left(\frac{\nu+2}{2}\right)\right)^2 .$$

But this equality must fail for every $\nu \geq 0$. Indeed, if $\nu=0$, the left side of (2.10) vanishes, while the right side is 2. If ν is positive, one side of (2.10) is an integer, while the other side is a rational multiple of π. Thus the assumption that F_ν has no zeros yields a contradiction, and Lemma 2.1 is proved. ∎

We can now give the

Proof of Theorem 2.2. Since for each pair (ν,n), the Padé numerator $Q_{\nu,n}(z)$ and Padé denominator $P_{\nu,n}(z)$ have no common factors, it suffices to show that for each fixed ν, the polynomials $P_{\nu,n}(z)$ have zeros of the form (2.4). Using the representation (1.3) the following integral formula can be derived:

$$(2.11)\quad (n+\nu)!\, P_{\nu,n}(z) = \int_0^\infty e^{-t}(t+z)^n t^\nu dt \quad , \quad (0 \leq t < +\infty) .$$

Letting $z = n + \sqrt{n}\, w$ and making the change of variables $t=\sqrt{n}\, u$, $0 \leq u < +\infty$, in (2.11) we find that

$$(2.12)\quad (n+\nu)!\, P_{\nu,n}(n+\sqrt{n}\, w) = n^{\frac{2n+\nu+1}{2}} \int_0^\infty e^{-\sqrt{n}\, u}\left\{1 + \frac{w+u}{\sqrt{n}}\right\}^n u^\nu du.$$

The logarithm of the integrand above is, for u and w fixed and n large,

$$\left(\sqrt{n}\, w - \frac{w^2}{2}\right) - wu - \frac{u^2}{2} + \nu \ln u + O\left(\frac{1}{\sqrt{n}}\right) ,$$

and so

$$\lim_{n\to\infty} e^{-\sqrt{n}\, u}\left\{1 + \frac{w+u}{\sqrt{n}}\right\}^n u^\nu / e^{\sqrt{n}\, w - w^2/2} = u^\nu e^{-wu-u^2/2} .$$

Now the proof given by Newman and Rivlin [4] can be adapted here to show, using the Lebesgue Dominated Convergence Theorem, that

$$(2.13)\quad \lim_{n\to\infty} \frac{(n+\nu)!\ P_{\nu,n}(n+\sqrt{n}\ w)}{e^{\sqrt{n}\ w-w^2/2}\ n^{\frac{2n+\nu+1}{2}}} = \int_0^\infty u^\nu e^{-wu-u^2/2}du =: F_\nu(w) \quad ,$$

the convergence being uniform on compact subsets of the w-plane. Since, by Lemma 2.1, $F_\nu(w)(\neq 0)$ has a finite zero, say w_ν, Hurwitz's Theorem implies that $P_{\nu,n}(n+\sqrt{n}\ w)$ possesses a zero, say $w=w_{\nu,n}$, such that $w_{\nu,n}\to w_\nu$ as $n\to\infty$. This means $P_{\nu,n}(z)$ has a zero of the form (2.4). ▌

Concerning pole-free sectors for the Padé approximants $R_{\nu,n}(z)$ the following is known:

THEOREM 2.3 (Saff, Varga [9], [11]). *For every $\nu\geq 0$, $n\geq 2$, the Padé approximant $R_{\nu,n}(z)$ for e^{-z} has no poles in the infinite sector*

$$(2.14)\quad S_{\nu,n} := \{z : |\arg z| \leq \cos^{-1}(\tfrac{n-\nu-2}{n+\nu})\} \ .$$

Furthermore, for any fixed σ, $0<\sigma<+\infty$, each element in the sequence of approximants $\{R_{\nu_j,n_j}(z)\}_{j=1}^\infty$ satisfying

$$(2.15)\quad \lim_{j\to\infty} n_j = +\infty \ , \ \lim_{j\to\infty} \nu_j/n_j = \sigma \ , \text{ and } (\frac{\nu_j+1}{n_j-1}) \geq \sigma \ ,$$

for all $j\geq 1$, is pole-free in the infinite sector

$$(2.16)\quad S_\sigma := \{z : |\arg z| \leq \cos^{-1}(\tfrac{1-\sigma}{1+\sigma})\} \ ,$$

and S_σ is the largest sector of the form $|\arg z| \leq \mu$, $\mu>0$, which is devoid of all poles of any sequence of approximants $\{R_{\nu_j,n_j}(z)\}_{j=1}^\infty$ satisfying (2.15).

In particular, for any (fixed) $\sigma>0$, S_σ is the largest pole-free sector of the form $|\arg z| \leq \mu$, $\mu>0$, for the sequence $\{R_{[\sigma n],n}(z)\}_{n=1}^{\infty}$, where $[\cdot]$ denotes the greatest integer function. This fact has an interesting geometric interpretation as explained in [9].

Using Theorems 2.2, 2.3, and the results in [11], we can deduce the following new result:

THEOREM 2.4. A necessary and sufficient condition that a sequence of Padé approximants $\{R_{\nu_k,n_k}(z)\}_{k=1}^{\infty}$, with $n_k \to \infty$, be pole-free in some infinite sector $|\arg z| < \mu$, $\mu > 0$, is that

$$(2.17) \quad \liminf_{k\to\infty} \nu_k/n_k > 0 \quad .$$

Proof. The sufficiency part follows immediately from Theorem 2.3. To prove necessity assume that (ν_k, n_k) is a sequence such that $n_k \to \infty$ and $\liminf_{k\to\infty} \nu_k/n_k = 0$. Our aim is to show that for every $\mu > 0$, there are infinitely many poles of the sequence $\{R_{\nu_k,n_k}(z)\}_{k=1}^{\infty}$ in the sector $|\arg z| < \mu$. For this purpose let $\{(\nu_j, n_j)\}_{j=1}^{\infty}$ denote a subsequence of $\{(\nu_k, n_k)\}_{k=1}^{\infty}$ for which $\lim_{j\to\infty} \nu_j/n_j = 0$. We consider two separate cases:

Case 1: If some subsequence of $\{\nu_j\}_{j=1}^{\infty}$ is bounded, then there is evidently a subsequence $\{(\nu_\ell, n_\ell)\}_{\ell=1}^{\infty}$ of $\{(\nu_j, n_j)\}_{j=1}^{\infty}$ for which ν_ℓ is constant, say $\nu_\ell = \nu$ for all $\ell \geq 1$, and for which $\lim_{\ell\to\infty} n_\ell = \infty$. But as a consequence of Theorem 2.2, the sequence $\{R_{\nu,n_\ell}(z)\}_{\ell=1}^{\infty}$ has poles which asymptotically (as $n_\ell \to \infty$) lie on some parabola opening about the positive real axis. Therefore the sequence has infinitely many poles in any sector of the form $|\arg z| < \mu$, $\mu > 0$.

Case 2: If $\nu_j \to \infty$ as $j \to \infty$, and $\lim_{j\to\infty} \nu_j/n_j = 0$, then the result of Corollary 3.1 of [11] applied to the sequence $\{P_{\nu_j,n_j}(z)\}$ of Padé denominators for e^{-z} again shows that there is no pole-free sector of the form $|\arg z| < \mu$, $\mu>0$, for the sequence $\{R_{\nu_j,n_j}(z)\}_{j=1}^{\infty}$. ∎

The next theorem has application to stability questions and extends results in [3] and [18].

THEOREM 2.5 (Saff, Varga [9]). *If* $n\leq\nu+4$, *the Padé approximant* $R_{\nu,n}(z)$ *for* e^{-z} *has all its poles in the open left half-plane.*

The above theorem is sharp in the sense that the approximant $R_{0,5}(z)$, for which $n=\nu+5$, does in fact have a pole in the right half-plane. However the following assertion can be made with regard to diagonal sequences of the table (1.4) of the form $\{R_{n-\tau,n}(z)\}_{n=\tau}^{\infty}$, $\tau\geq 5$:

THEOREM 2.6 (Saff, Varga [9]). *For any integer* $\tau\geq 5$, *there exists an integer* $m=m(\tau)$ *such that the approximants* $\{R_{n-\tau,n}(z)\}_{n=m}^{\infty}$ *have all their poles in the open left half-plane.*

3 Geometric convergence of Padé approximants in unbounded regions

In this section we discuss results concerning geometric convergence of Padé approximants on the nonnegative ray $[0,+\infty)$, and on infinite sectors of the form $|\arg z| \leq \mu$, $\mu>0$. First we set

$$(3.1)\quad \eta_{\nu,n}:=||e^{-x}-R_{\nu,n}(x)||_{L_\infty[0,+\infty)} \quad .$$

Notice that when $\nu>n$, we have $\eta_{\nu,n}=|e^{-\infty}-R_{\nu,n}(\infty)| = \infty$. When $\nu\leq n$ the following estimates are known:

THEOREM 3.1 (Saff, Varga, Ni [12]). *For any nonnegative integers* ν *and* n *with* $0\leq\nu\leq n$, *there holds*

$$(3.2)\qquad \frac{\gamma}{2^{n-\nu}\binom{n}{\nu}\,(n+1)^2} < \eta_{\nu,n} \leq \frac{1}{2^{n-\nu}\binom{n}{\nu}} \quad ,$$

where γ *is a positive constant independent of* ν *and* n .

To state the next theorem we need the function $g(\beta)$ defined for $0\leq\beta\leq 1$ by

$$(3.3)\qquad g(\beta) := \frac{\beta^{\beta}(1-\beta)^{1-\beta}}{2^{1-\beta}} \quad , \; 0<\beta<1 \quad , \; g(0):=1/2 \; , \; g(1):=1 \quad .$$

THEOREM 3.2 (Saff, Varga, Ni [12]). *Let* $\{\nu(n)\}_{n=1}^{\infty}$ *be a sequence of nonnegative integers with* $0\leq\nu(n)\leq n$ *for all* n , *and satisfying* $\lim_{n\to\infty} \nu(n)/n = \beta$. *Then*

$$(3.4)\qquad \lim_{n\to\infty} \eta_{\nu(n),n}^{1/n} = g(\beta) \quad .$$

As $\min_{0\leq\beta\leq 1} g(\beta) = g(1/3) = 1/3$, it follows from the above theorem that for *any* sequence $\{\nu(n)\}_{n=1}^{\infty}$, there holds

$$\liminf_{n\to\infty} \eta_{\nu(n),n}^{1/n} \geq \frac{1}{3} \quad ,$$

with equality possible for the sequence $\{R_{[n/3],n}(x)\}_{n=1}^{\infty}$. Indeed numerical computations appear to indicate that for each fixed n the smallest error $\eta_{\nu,n}$, $\nu=0,1,2,\ldots$, occurs when $\nu=[n/3]$. Another consequence of Theorem 3.2 is stated in

THEOREM 3.3 (Saff, Varga, Ni [12]). *A necessary and sufficient condition that a sequence of Padé approximants* $\{R_{\nu(n),n}(x)\}_{n=1}^{\infty}$ *converges geometrically in the uniform norm to* e^{-x} *on* $[0,+\infty)$ *is that*

$$(3.5)\qquad \limsup_{n\to\infty} \frac{\nu(n)}{n} < 1 \quad .$$

Concerning geometric convergence in the uniform norm over infinite sectors we shall prove the following new result:

THEOREM 3.4. A necessary and sufficient condition that a sequence of Padé approximants $\{R_{\nu(n),n}(z)\}_{n=1}^{\infty}$ converges geometrically in the uniform norm to e^{-z} in some infinite sector $S_\mu := \{z : |\arg z| \le \mu\}$, $\mu>0$, is that

$$(3.6)\quad 0 < \liminf_{n\to\infty} \frac{\nu(n)}{n} \le \limsup_{n\to\infty} \frac{\nu(n)}{n} < 1 \quad .$$

Proof. That condition (3.6) is sufficient to ensure geometric convergence in some S_μ , $\mu>0$, is proved in [12]. To demonstrate necessity we assume that for some $\mu>0$, the sequence $\{R_{\nu(n),n}(z)\}_{n=1}^{\infty}$ satisfies

$$(3.7)\quad \limsup_{n\to\infty} \|e^{-z} - R_{\nu(n),n}(z)\|_{L_\infty(S_\mu)}^{1/n} < 1 \quad .$$

Since S_μ contains the ray $[0,+\infty)$, it follows from Theorem 3.3 that $\limsup_{n\to\infty} \nu(n)/n < 1$. Furthermore, as (3.7) evidently implies that for n large enough, the poles of the sequence $\{R_{\nu(n),n}(z)\}$ must omit the sector S_μ , Theorem 2.4 implies $\liminf_{n\to\infty} \nu(n)/n > 0$. ∎

Concerning estimates for the size of the sector S_μ of geometric convergence for a sequence satisfying (3.6), the reader is referred to [12]. We remark that although no column of the table (1.4) converges geometrically to e^{-z} in an infinite sector, each column does, in fact, converge geometrically to e^{-z} on an unbounded parabolic region (see [10]).

Of course the poles of the Padé approximants to e^{-z} are, in general, not all real. For computational purposes it is sometimes desirable to deal with rational approximations whose poles are all real and coincident. In [7] it is shown that there exists a sequence of rational functions of the form

$$r_n(x) = \frac{p_{n-1}(x)}{(1+\frac{x}{n})^n}, \quad \deg p_{n-1} \leq n-1, \quad n=1,2,\ldots,$$

such that

$$||e^{-x} - r_n(x)||_{L_\infty[0,+\infty)} = O(\frac{n}{2^n}) \quad \text{as} \quad n\to\infty .$$

Some further properties of this sequence are discussed in [7].

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