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ON THE ZEROS AND POLES OF PADÉ APPROXIMANTS TO e^z. II.

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In this paper, we continue our study of the location of the zeros and poles of general Padé approximants to e^z. We state and prove here two new results on improved estimates for the zeros of general Padé approximants $R_{n,\nu}(z)$ to e^z, and state results on the asymptotic location of the normalized zeros and poles for certain sequences of Padé approximants to e^z.

1 Introduction

A number of recent papers (cf. [1, 4, 6, 9, 15]) have been concerned with Padé rational approximations of e^z because of applications to the numerical analysis of methods for solving certain systems of ordinary differential equations. The purpose of this present paper is to continue our study [9] on the zeros and poles of general Padé approximants to e^z. In particular, for every Padé approximant we determine a "close-to-sharp" annulus, having center at $z = 0$, containing all the zeros and poles of this approximant. These results will be described in §2, with their proofs being given in §3.

In this paper, we also state more precise information about the asymptotic distribution of the zeros and poles for specific sequences of Padé approximants to e^z. What has motivated this work is an article by Szegö [13], which considers the zeros of the partial sums $s_n(z) := \sum_{k=0}^{n} z^k/k!$ of the Maclaurin expansion of e^z. Szegö [13] showed that $s_n(nz)$ has all its zeros in $|z| \leq 1$ for every $n \geq 1$, and that $\hat{z}$ is a limit point of zeros of $\{s_n(nz)\}_{n=1}^{\infty}$ iff

(1.1) $\quad |\hat{z}\, e^{1-\hat{z}}| = 1$ and $|\hat{z}| \leq 1$.

(This result was also obtained later independently by Dieudonné [3].)

The connection of Szegö's result with Padé approximations of e^z is evident in that $s_n(z)$ is the $(n, 0)$-th Padé approximant to e^z. Our new results, giving sharp generalizations of Szegö's result to the asymptotic distribution of zeros of more general sequences of Padé approximants to e^z, will be stated explicitly in §2, but their proofs, being lengthy, will appear elsewhere. For the remainder of this section, we introduce necessary notation and cite needed known results.

Let π_m denote the set of all polynomials in the variable z having degree at most m, and let $\pi_{n,\nu}$ be the set of all complex rational functions $r(z)$ of the form

$$r(z) = \frac{p(z)}{q(z)}, \text{ where } p \in \pi_n,\ q \in \pi_\nu, \text{ and } q(0) = 1.$$

Then, the (n,ν)-th Padé approximation to e^z is defined as that element $R_{n,\nu}(z) \in \pi_{n,\nu}$ for which

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

In explicit form, it is known [8, p. 245] that

$$R_{n,\nu}(z) = P_{n,\nu}(z)/Q_{n,\nu}(z);$$

where

$$(1.2)\quad P_{n,\nu}(z) := \sum_{j=0}^{n} \frac{(n+\nu-j)!\ n!\ z^j}{(n+\nu)!\ j!\ (n-j)!},$$

and

$$(1.3)\quad Q_{n,\nu}(z) := \sum_{j=0}^{\nu} \frac{(n+\nu-j)!\ \nu!\ (-z)^j}{(n+\nu)!\ j!\ (\nu-j)!}.$$

We shall refer to the polynomials $P_{n,\nu}(z)$ and $Q_{n,\nu}(z)$ respectively as the <u>Padé numerator</u> and <u>Padé denominator</u> of type (n, ν) for e^z.

Generally, one is interested in both the zeros and the poles of the Padé approximants $R_{n,\nu}(z)$. However, since the polynomials of (1.2) and (1.3) satisfy the obvious relation

$$(1.4)\quad Q_{n,\nu}(z) = P_{\nu,n}(-z),$$

it suffices then to investigate only the <u>zeros</u> of the Padé approximants $R_{n,\nu}(z)$, or equivalently, the zeros of the Padé numerator $P_{n,\nu}(z)$.

The approximants $R_{n,\nu}(z)$ are typically displayed in the following infinite array, known as the <u>Padé table for</u> e^z:

$$(1.5)\quad \begin{bmatrix} R_{0,0}(z) & R_{1,0}(z) & R_{2,0}(z) & \cdots \\ R_{0,1}(z) & R_{1,1}(z) & R_{2,1}(z) & \cdots \\ R_{0,2}(z) & R_{1,2}(z) & R_{2,2}(z) & \cdots \\ \vdots & \vdots & \vdots & \end{bmatrix}$$

Note that the first row $\{R_{n,0}(z)\}_{n=0}^{\infty}$ of the Padé table for e^z is, from (1.2), simply the sequence of partial sums $\{s_n(z) = \sum_{k=0}^{n} z^k/k!\}_{n=0}^{\infty}$ of e^z.

Essential for the statements and proofs of our main results are the following recent results on zeros of Padé approximants for e^z.

THEOREM 1.1. (Saff and Varga [9], [11], [12]). <u>For every</u> $\nu \geq 0$, $n \geq 2$, <u>the Padé approximant</u> $R_{n,\nu}(z)$ <u>for</u> e^z <u>has all its zeros in the infinite sector</u>

$$(1.6)\quad \mathcal{S}_{n,\nu} := \{z: |\arg z| > \cos^{-1}(\frac{n-\nu-2}{n+\nu})\}.$$

<u>Furthermore, on defining generically the infinite sector</u> $\mathcal{S}_\lambda$, $\lambda \geq 0$, by

$$(1.7)\quad \mathcal{S}_\lambda := \{z: |\arg z| > \cos^{-1}(\frac{1-\lambda}{1+\lambda})\},$$

<u>consider any sequence of Padé approximants</u> $\{R_{n_j,\nu_j}(z)\}_{j=1}^{\infty}$ <u>satisfying</u>

$$(1.8)\quad \lim_{j\to\infty} n_j = +\infty, \text{ and } \lim_{j\to\infty} \frac{\nu_j}{n_j} = \sigma,$$

for any σ *with* $0 < \sigma < \infty$. *Then, for any* ϵ with $0 < \epsilon < \sigma$, $\{R_{n_j,\nu_j}(z)\}_{j=1}^{\infty}$ *has infinitely many zeros in* $\mathcal{S}_{\sigma-\epsilon}$ *and only finitely many zeros in the complement of* $\mathcal{S}_{\sigma-\epsilon}$, *and* $\mathcal{S}_{\sigma}$ *is the smallest sector of the form* $|\arg z| > \mu$, $\mu > 0$, *with this property*.

THEOREM 1.2. (Saff and Varga [9]). *If* $1 < n < 3\nu + 4$, *then all the zeros of the Padé approximant* $R_{n,\nu}(z)$ *for* e^z *lie in the half-plane*

(1.9) $\operatorname{Re} z < n - \nu - 2.$

2 *Statements of New Results*

We list and discuss our main results in this section. Our first results give estimates for the zeros of *general* Padé approximants $R_{n,\nu}(z)$, which extend the results of Theorem 1.2 of §1.

THEOREM 2.1. *For any* $n \geq 1$ *and any* $\nu \geq 0$, *all the zeros of the Padé approximant* $R_{n,\nu}(z)$ *satisfy*

(2.1) $\operatorname{Re} z < n - \nu.$

THEOREM 2.2. *For any* $n \geq 1$ *and any* $\nu \geq 0$, *all the zeros of the Padé approximant* $R_{n,\nu}(z)$ *lie in the annulus*

(2.2) $(n+\nu)\mu < |z| < n+\nu+4/3 \quad (\mu \doteq 0.278\ 465),$

where μ *is the unique positive root of* $\mu e^{1+\mu} = 1$. *Moreover, the constant* μ *in (2.2) is best possible in the sense that*

$$\mu = \inf_{\substack{n\geq 1\\ \nu\geq 0}} \left\{\frac{|z|}{(n+\nu)} : R_{n,\nu}(z) = 0\right\}.$$

We remark that while the first inequality of (2.2) of Theorem 2.2 is best possible in the above sense, the upper bound of (2.2) may not be best possible. In any event, because $R_{1,\nu}(z)$ has its sole zero at $z = -(\nu+1)$, we have

$$\sup_{n\geq 1,\ \nu\geq 0} \{|z| - (n+\nu) : R_{n,\nu}(z) = 0\} \geq 0$$

and thus, the constant 4/3 in (2.2) can however be decreased at most to zero. In fact, the Kakeya-Eneström Theorem (cf. [5, p. 106, Ex. 2]) directly gives that all the zeros of $s_n(z)$ lie in $|z| \leq n$, which sharpens the last inequality of (2.2) of Theorem 2.2 for the case $\nu = 0$. However, applying the Kakeya-Eneström Theorem to the general Padé numerator $P_{n,\nu}(z)$ gives only that $P_{n,\nu}(z)$ has all its zeros in $|z| \leq n(\nu+1)$ which, except in essentially trivial cases, gives a worse upper bound than that of the last inequality of (2.2) of Theorem 2.2.

Note that because of the relation (1.4), the inequalities of (2.2) of Theorem 2.2 hold for the zeros as well as for the poles of $R_{n,\nu}(z)$. Thus, given any compact subset Ω of the complex plane $\mathbb{C}$, there is a constant $\gamma > 0$, depending only on the geometry of Ω, such that all zeros and poles of any Padé approximant $R_{n,\nu}(z)$ lie outside of Ω if $(n+\nu) \geq \gamma$.

To describe the remaining results, for any σ with $0 < \sigma < +\infty$, define the points

$$(2.3) \quad z_\sigma^{\pm} := \{(1-\sigma) \pm 2\sqrt{\sigma}\, i\}/(1+\sigma),$$

which have modulus unity, and consider the complex plane $\mathbb{C}$ slit along the two rays

$$\mathcal{R}_\sigma := \{z : z = z_\sigma^+ + i\tau \text{ or } z = z_\sigma^- - i\tau,\ \tau \geq 0\},$$

as shown in Figure 1. Now, the function

$$(2.4) \quad g_\sigma(z) := \sqrt{1 + z^2 - 2z\left(\frac{1-\sigma}{1+\sigma}\right)}$$

has z_σ^+ and z_σ^- as branch points, which

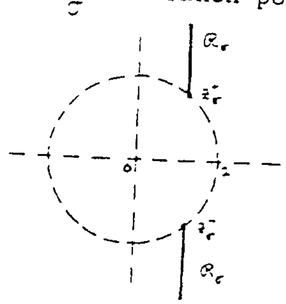

Figure 1

are the finite extremities of $\mathcal{R}_\sigma$. On taking the principal branch for the square root, i.e., on setting $g_\sigma(0) = 1$ and extending g_σ analytically on this doubly slit domain $\mathbb{C}\backslash\mathcal{R}_\sigma$, then g_σ is analytic and single-valued on $\mathbb{C}\backslash\mathcal{R}_\sigma$. Next, it can be verified that $1 \pm z + g_\sigma(z)$ does not vanish on $\mathbb{C}\backslash\mathcal{R}_\sigma$. Thus, we define, respectively, $(1 + z + g_\sigma(z))^{\frac{2}{1+\sigma}}$ and $(1 - z + g_\sigma(z))^{\frac{2\sigma}{1+\sigma}}$ by requiring that their values at $z = 0$ be $2^{\frac{2}{1+\sigma}}$ and $2^{\frac{2\sigma}{1+\sigma}}$, and by analytic continuation. These functions are also analytic and single-valued in $\mathbb{C}\backslash\mathcal{R}_\sigma$. With these conventions, we set

$$(2.5)\quad w_\sigma(z) := \frac{4\sigma^{\left(\frac{\sigma}{1+\sigma}\right)} z\, e^{g_\sigma(z)}}{(1+\sigma)(1+z+g_\sigma(z))^{\frac{2}{1+\sigma}}(1-z+g_\sigma(z))^{\frac{2\sigma}{1+\sigma}}},$$

$$0 < \sigma < +\infty,$$

and it follows that w_σ is analytic and single-valued on $\mathbb{C}\backslash\mathcal{R}_\sigma$. Next, on letting $\sigma \to 0$ in (2.5), we obtain that $w_0(z) := \lim_{\sigma\to 0} w_\sigma(z)$ satisfies

$$(2.5')\quad w_0(z) = z\, e^{1-z},$$

for $\text{Re } z \le 1$.

With these definitions, we state the following results, whose proofs will appear elsewhere.

THEOREM 2.3. <u>For any σ with $0 \le \sigma < \infty$, consider any sequence of Padé approximants $\{R_{n_j,\nu_j}(z)\}_{j=1}^\infty$ for e^z for which</u>

$$(2.6)\quad \lim_{j\to\infty} n_j = +\infty, \text{ and } \lim_{j\to\infty} \frac{\nu_j}{n_j} = \sigma.$$

<u>Then, $\hat{z}$ is a limit point of zeros of the normalized Padé approximants $\{R_{n_j,\nu_j}((n_j+\nu_j)z)\}_{j=1}^\infty$ iff $\hat{z}$ belongs to the curve</u>

$$(2.7)\quad D_\sigma := \{z \in \overline{\mathcal{S}}_\sigma : |w_\sigma(z)| = 1 \text{ and } |z| \le 1\},$$

where $\overline{\mathfrak{S}}_\sigma$ denotes the closure of $\mathfrak{S}_\sigma$ (cf. (1.7)).

We first remark that the special case of Theorem 2.3 with $\sigma = 0$ and, in addition, with $\nu_j = 0$ and $n_j = j$ for all $j \geq 1$, reduces to Szegö's result (cf. (1.1) and (2.7)) since $\overline{\mathfrak{S}}_0 = \mathbb{C}$, and since the normalized approximants $\{R_{j,0}(jz)\}_{j=1}^{\infty}$ are just $\{s_n(nz)\}_{n=1}^{\infty}$.

We illustrate this special case of $\sigma = 0$ of Theorem 2.3 by graphing respectively, in Figures 2 and 3, the twelve zeros of $s_{12}(12z)$ and the twenty-four zeros of $s_{24}(24z)$, along with D_0, indicated by the solid curve.

Similarly, for the choice $\nu_j = j = n_j$ for all $j \geq 1$, (2.6) is satisfied for $\sigma = 1$, and in this case, Figures 4 and 5 indicate the curve D_1, along with, respectively, the twelve zeros of the polynomial $P_{12,12}(24z)$, and the twenty-four zeros of the polynomial $P_{24,24}(48z)$. Next, we remark that the curve D_1, after rotations of $\pi/2$, form the boundaries of the eye-shaped domain consider by Olver [7, p. 336] in his asymptotic expansions of Bessel functions. That such a connection exists is not surprising, since the diagonal Padé numerators $P_{n,n}(z)$ satisfy $P_{n,n}(2iz) = n!(2z)^n e^{iz}(\pi z/2)^{1/2}\{(-1)^n J_{-(n+1/2)}(z) - iJ_{n+1/2}(z)\}/(2n)!$.

To further illustrate the result of Theorem 2.3, we note that the choice $\nu_j = j$, $n_j = 3j$ for all $j \geq 1$ satisfies (2.6) with $\sigma = 1/3$, and Figures 6 and 7 show $D_{1/3}$, along with the twelve zeros of $P_{12,4}(16z)$ and the twenty-four zeros of the polynomial $P_{24,8}(32z)$. Thus, we see from Figures 2-7 that Theorem 2.3 quite accurately predicts the zeros of $P_{n,\nu}((n+\nu)z)$, even for relatively small values of n and ν.

With the relationship of (1.4), Theorem 2.3 can directly be used to deduce the limit points of the poles of $\{R_{n_j,\nu_j}((n_j+\nu_j)z)\}_{j=1}^{\infty}$. Specifically, we state

COROLLARY 2.4. *Let $\{R_{n_j,\nu_j}(z)\}_{j=1}^{\infty}$ be a sequence of Padé approximants to e^z satisfying (2.6) with $0 < \sigma < \infty$. Then $\hat{z}$ is a limit point of poles of $\{R_{n_j,\nu_j}((n_j+\nu_j)z)\}_{j=1}^{\infty}$ iff $\hat{z}$ belongs to the curve $-D_{1/\sigma}$ where (cf. (2.7))*

(2.8) $-D_{1/\sigma} := \{z : -z \in D_{1/\sigma}\}$.

Interestingly enough, the closed curve

(2.9) $J_\sigma := \{z: |w_\sigma(z)| = 1 \text{ and } |z| \le 1\}$

can be represented as the union

(2.10) $J_\sigma = D_\sigma \cup \{-D_{1/\sigma}\}, \; 0 < \sigma < \infty.$

Thus, the limit points of zeros and poles of $\{R_{n_j,\nu_j}((n_j+\nu_j)z)\}_{j=1}^{\infty}$ play a complementary role to one another. To illustrate this, consider the sequence of Padé approximants $\{R_{3m,m}(4m\,z)\}_{m=1}^{\infty}$, for which $\sigma = 1/3$. In Figure 8, we have graphed $D_{1/3}$ and $(-D_3)$, along with the 24 zeros and 8 poles of $R_{24,8}(32z)$, denoted respectively by *'s and □'s.

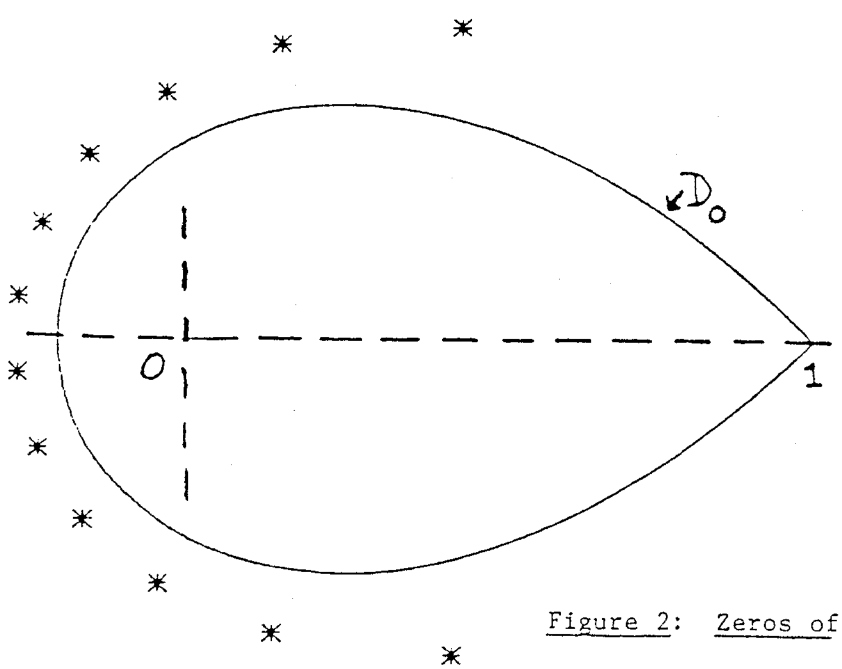

Figure 2: Zeros of $s_{12}(12z)$.

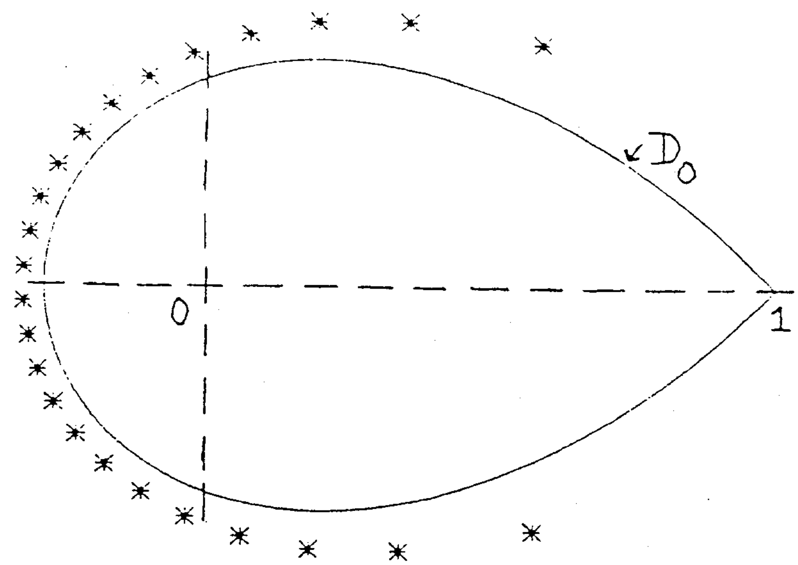

Figure 3: Zeros of $s_{24}(24z)$.

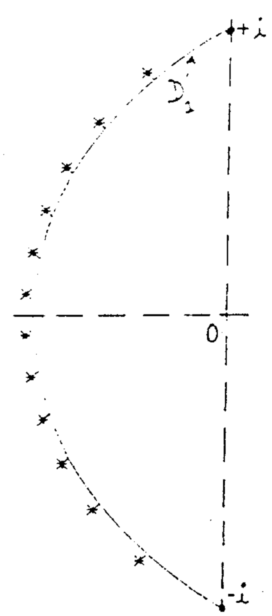

Figure 4: Zeros of $P_{12,12}(24z)$.

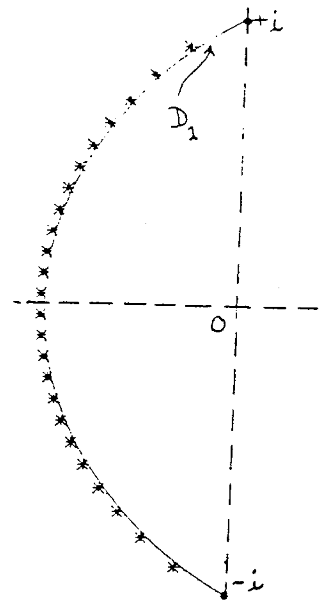

Figure 5: Zeros of $P_{24,24}(48z)$.

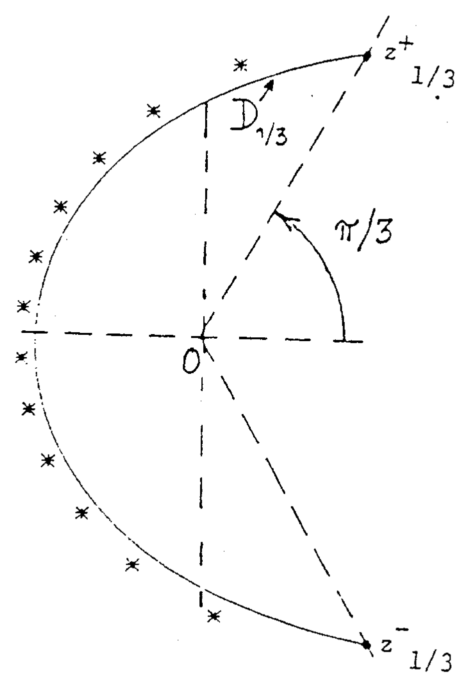

Figure 6: Zeros of $P_{12,4}(16z)$.

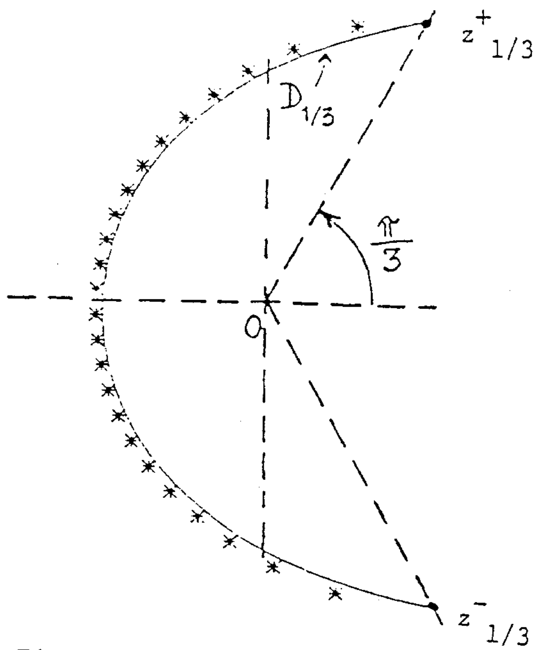

Figure 7: Zeros of $P_{24,8}(32z)$.

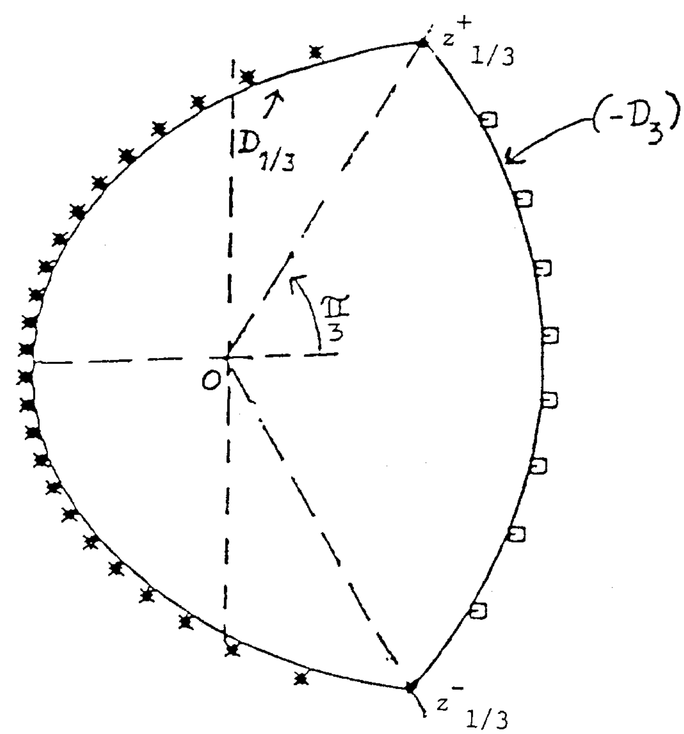

Figure 8: Zeros and Poles of $R_{24,8}(32z)$.

3 Proofs of Theorems 2.1 and 2.2

As in Saff-Varga [11], for any $n \geq 0$ and any $\nu \geq 0$, set

$$(3.1)\quad w_{n,\nu}(z) := e^{-z/2} z^{-(\frac{n+\nu}{2})} P_{n,\nu}(z),$$

where the Padé numerator $P_{n,\nu}(z)$ is defined in (1.2). In the case that $n+\nu$ is odd, $z^{-(\frac{n+\nu}{2})}$ denotes the principal branch of $z^{-(\frac{n+\nu}{2})}$. Then, as is known (cf. Olver [7, p. 260]), $w_{n,\nu}(z)$ satisfies Whittaker's equation

$$(3.2)\quad \frac{d^2 w(z)}{dz^2} = [\frac{1}{4} - \frac{k}{z} + \frac{\lambda}{z^2}]\, w(z),$$

with

$$(3.3)\quad k := \frac{n-\nu}{2}, \text{ and } \lambda := (\frac{n+\nu+1}{2})^2 - \frac{1}{4} = \frac{(n+\nu)(n+\nu+2)}{4}.$$

Proof of Theorem 2.1. If $\nu \geq n > 1$, then $3\nu + 4 > n > 1$, so that from (1.9) of Theorem 1.2, we have that any zero z of $P_{n,\nu}(z)$ satisfies

$$\operatorname{Re} z < n - \nu - 2,$$

which is stronger than the desired result (2.1) of Theorem 2.1. Similarly, if $n = 1$, the single zero of $P_{1,\nu}(z)$ is $z = -(\nu+1)$, which implies that

$$\operatorname{Re} z = n - \nu - 2,$$

and again (2.1) of Theorem 2.1 is satisfied.

For the remaining case $0 \leq \nu < n$, define

$$(3.4)\quad y_\tau(x) := w_{n,\nu}(\tau x),\ \tau \neq 0,\ 0 \leq x < \infty,$$

which, using (3.2), satisfies

$$(3.5)\quad \frac{d^2 y_\tau(x)}{dx^2} = \tau^2\{\frac{1}{4} - \frac{k}{\tau x} + \frac{\lambda}{\tau^2 x^2}\}\, y_\tau(x) =: p_\tau(x)\cdot y_\tau(x).$$

Next, choose τ to be a zero of $P_{n,\nu}$, i.e., $w_{n,\nu}(\tau) = 0 = y_\tau(1)$. If $\mathrm{Re}\,\tau \leq 0$, then by hypothesis $\mathrm{Re}\,\tau \leq 0 < n - \nu$, and (2.1) of Theorem 2.1 is trivially satisfied. Hence, assume that $\mathrm{Re}\,\tau > 0$, in which case $\bar{\tau}$ is also a distinct zero of $P_{n,\nu}$. Defining similarly

(3.6) $\quad y_{\bar{\tau}}(x) := w_{n,\nu}(\bar{\tau}x), \quad 0 \leq x < \infty,$

which satisfies

(3.7) $$\frac{d^2 y_{\bar{\tau}}(x)}{dx^2} = \bar{\tau}^2\left\{\frac{1}{4} - \frac{k}{\bar{\tau}x} + \frac{\lambda}{\bar{\tau}^2 x^2}\right\} y_{\bar{\tau}}(x) =: p_{\bar{\tau}}(x) y_{\bar{\tau}}(x),$$

it follows from (3.5) and (3.7) that for real a and b,

(3.8) $$\int_a^b (p_{\bar{\tau}}(x) - p_\tau(x))\, y_\tau(x) y_{\bar{\tau}}(x)\,dx$$
$$= \int_a^b \left\{y_\tau(x)\frac{d^2 y_{\bar{\tau}}(x)}{dx^2} - y_{\bar{\tau}}(x)\frac{d^2 y_\tau(x)}{dx^2}\right\}dx$$
$$= \left(y_\tau(x)\frac{dy_{\bar{\tau}}(x)}{dx} - y_{\bar{\tau}}(x)\frac{dy_\tau(x)}{dx}\right)\Bigg|_{x=a}^{x=b}.$$

Now, because $\mathrm{Re}\,\tau > 0$, we see from (3.1) that $y_\tau(x)$, $y_{\bar{\tau}}(x)$, and their derivatives tend to zero as $x \to +\infty$, and as $y_\tau(1) = y_{\bar{\tau}}(1) = 0$, the choice $a = 1$, $b = +\infty$ in (3.8) gives

$$\int_1^\infty (p_{\bar{\tau}}(x) - p_\tau(x)) y_\tau(x) y_{\bar{\tau}}(x)\,dx = 0.$$

Equivalently, using the definitions of p_τ and $p_{\bar{\tau}}$, we have that

$$(\bar{\tau} - \tau)\int_1^\infty \left\{\frac{\tau + \bar{\tau}}{4} - \frac{k}{x}\right\} |y_\tau(x)|^2\,dx = 0,$$

since $\overline{y_\tau(x)} = y_{\bar{\tau}}(x)$. But as $(\tau - \bar{\tau}) \neq 0$, this reduces to

$$(3.9)\quad \int_1^\infty \left\{\frac{\operatorname{Re}\tau}{2} - \frac{k}{x}\right\} |y_\tau(x)|^2 \, dx = 0.$$

Clearly, the term $g(x) := \frac{\operatorname{Re}\tau}{2} - \frac{k}{x}$, which is monotone increasing on $[1, +\infty)$ and positive at infinity, cannot be positive for all $x \geq 1$, as this would contradict (3.9). Thus, $g(1) = \frac{\operatorname{Re}\tau}{2} - k < 0$ which implies from (3.3) that $\operatorname{Re}\tau < 2k = n - \nu$, the desired result of (2.1) of Theorem 2.1. ∎

For the proof of Theorem 2.2, we need the following

LEMMA 3.1. *For any* $n \geq 1$, *and any* $\nu \geq 0$, *let* τ *be any maximal zero of* $P_{n,\nu}(z)$, *i.e.*,

$$(3.10)\quad P_{n,\nu}(\tau) = 0 \text{ and } |\tau| = \max\{|z| : P_{n,\nu}(z) = 0\}.$$

Then,

$$(3.11)\quad \operatorname{Re}\tau \geq -(\nu + 1).$$

Proof. First, it can be verified from (1.2) that $P_{n,\nu}(z)$ satisfies the differential equation

$$(3.12)\quad n\, P_{n,\nu}(z) = (z + n + \nu)\, P'_{n,\nu}(z) - z\, P''_{n,\nu}(z).$$

Next, it is known (cf. Saff-Varga [10]) that all the zeros of $P_{n,\nu}(z)$ are simple. With τ a maximal zero of $P_{n,\nu}(z)$, define, for any $n > 1$,

$$(3.13)\quad T := \tau - 2(n-1)\frac{P'_{n,\nu}(\tau)}{P''_{n,\nu}(\tau)}.$$

By definition, $P_{n,\nu}(z)$ has no zeros in $|z| > |\tau|$. Hence, using a result of Laguerre (cf. Szegö [14, p. 117]), T must lie in $|z| \leq |\tau|$, and, because $P_{n,\nu}(\tau) = 0$, equations (3.12) and (3.13) give that $T = \tau - \frac{2(n-1)\tau}{(\tau + n + \nu)}$. Then, a short calculation shows that $|T| \leq |\tau|$ implies (3.11) for any $n > 1$, any $\nu \geq 0$. If $n = 1$, the sole zero of $P_{1,\nu}(z)$ is $-(\nu + 1)$, which also satisfies (3.11). ∎

Proof of Theorem 2.2. We first establish the second inequality of (2.2) of Theorem 2.2. Let τ be a maximal zero (cf. (3.10)) of $P_{n,\nu}(z)$. If τ is real, then τ is evidently negative since $P_{n,\nu}(z)$ has only positive coefficients, and thus, applying Lemma 3.1, we have $|\tau| \le 1 + \nu \le n + \nu$. But as τ is a maximal zero of $P_{n,\nu}(z)$, then $|z| \le n + \nu$ for any zero of $P_{n,\nu}$, which satisfies the second inequality of (2.2) of Theorem 2.2.

Let τ then be any non-real maximal zero of $P_{n,\nu}(z)$ with $\operatorname{Im} \tau > 0$. With $w_{n,\nu}(z)$ defined in (3.1), set

(3.14) $y(x) := w_{n,\nu}(\tau(1 + \gamma x)), \ 0 \le x < \infty,$

where γ is a constant, to be selected later, such that

(3.15) $\operatorname{Re}(\tau\gamma) > 0.$

From (3.2), we see that y satisfies

(3.16) $$\frac{d^2y(x)}{dx^2} = (\tau\gamma)^2\left\{\frac{1}{4} - \frac{k}{\tau(1+\gamma x)} + \frac{\lambda}{\tau^2(1+\gamma x)^2}\right\}y(x) =: p(x)y(x).$$

Since $\bar{\tau}$ is also a maximal zero of $P_{n,\nu}(z)$, we also consider

(3.17) $\overline{y(x)} = w_{n,\nu}(\bar{\tau}(1+\bar{\gamma}x)), \ 0 \le x < \infty,$

which satisfies

(3.18) $$\frac{d^2\overline{y(x)}}{dx^2} = \overline{p(x)}\ \overline{y(x)}.$$

As before (cf. (3.8)), we similarly have that

$$\int_a^b (\overline{p(x)} - p(x))|y(x)|^2dx = \left(y(x)\frac{d\overline{y(x)}}{dx} - \overline{y(x)}\ \frac{dy(x)}{dx}\right)\Big|_{x=a}^{x=b}.$$

Because of (3.15) and (3.1), $y(x)$, $\overline{y(x)}$, and their derivatives tend to zero as $x \to +\infty$, and as $y(0) = \overline{y(0)} = 0$, the choice $a = 0$ and $b = +\infty$ in the above expression then gives

(3.19) $$\int_0^\infty (\overline{p(x)} - p(x))\ |y(x)|^2dx = 0.$$

Now, $p(x) - \overline{p(x)}$ is, purely imaginary, and using (3.16),

$$(3.20)\quad \frac{p(x)-\overline{p(x)}}{2i} = \frac{\operatorname{Im}\{(\tau\gamma)^2|1+\gamma x|^4 - |1+\gamma x|^2(1+\bar{\gamma}x)4k\tau\gamma^2 + 4\lambda\gamma^2(1+\bar{\gamma}x)^2\}}{4|1+\gamma x|^4}.$$

Because of (3.19), note that the numerator of the right side of (3.20) cannot be of one sign for all $0 \le x < \infty$. Writing $\tau = \rho e^{i\theta}$ with $0 < \theta < \pi$, we choose $\gamma := \frac{1}{\rho} e^{-i\theta/2}$, so that (3.15) is satisfied. With this choice of γ, the numerator of (3.20) can be written, after some algebraic manipulations, as the product $2\rho^{-4} \sin \frac{\theta}{2} \cdot \sigma_4(x)$, where $\sigma_4(x)$, a quartic polynomial, is defined by

$$(3.21)\quad \begin{cases} \sigma_4(x) := x^4[\cos \frac{\theta}{2}] + x^3[4\rho \cos^2 \frac{\theta}{2} - 2k] \\ + x^2[(2\rho^2 - 4k\rho)\cos \frac{\theta}{2} + 4\rho^2\cos^3 \frac{\theta}{2}] + x[4\rho^3\cos^2 \frac{\theta}{2} - 2k\rho^2 - 4\lambda\rho] \\ + [\rho^4 - 4\lambda\rho^2]\cos \frac{\theta}{2}. \end{cases}$$

As before, σ_4 cannot be of one sign on $[0, +\infty)$ because of (3.19).

To complete the proof of the second inequality of (2.2) of Theorem 2.2, assume on the contrary that $\rho = |\tau| \ge n + \nu + 4/3$. Using the definitions of (3.3) and in particular the result of Lemma 3.1, a lengthy calculation (which we omit) shows that $\sigma_4(x) := \sum_{i=0}^{4} \beta_i x^i$ has only positive coefficients β_i, $0 \le i \le 4$, a contradiction. Thus, $|\tau| < n + \nu + 4/3$, and as τ is a maximal zero of $P_{n,\nu}(z)$, all zeros of $P_{n,\nu}(z)$ necessarily satisfy $|z| < n + \nu + 4/3$, the desired second inequality of (2.2) of Theorem 2.2.

We now establish the first inequality of (2.2). For the partial sums $s_n(z) := \sum_{k=0}^{n} z^k/k!$ of the Maclaurin expansion for e^z, it is known (cf. Buckholtz [2]) that, for any $n \ge 1$, any zero $\hat{z}$ of the normalized polynomial $s_n(nz)$ satisfies

(3.22) $|\hat{z}e^{1-\hat{z}}| > 1$ and $|\hat{z}| < 1$,

i.e., as Figures 2 and 3 show, $\hat{z}$ lies outside D_0 but in the unit disk. It is easy to verify (cf. Figures 2 and 3) that the point ζ in the unit disk satisfying $|\zeta e^{1-\zeta}| = 1$ which is closest to the origin is the real point $\zeta = -\mu, \mu > 0$, where $\mu e^{1+\mu} = 1$, and μ is given approximately by $\mu \doteq 0.278\ 465$. Hence, for any $n \geq 1$, any zero z of $s_n(z)$ from (3.22) satisfies

(3.23) $|z| > n\mu$.

Since $s_n(z) = P_{n,0}(z)$, then (3.23) gives the desired first inequality of (2.2) of Theorem 2.2 for the case $\nu = 0$.

Next, on defining the "reciprocal" Padé numerators:

(3.24) $P^*_{n,\nu}(z) := z^n P_{n,\nu}(1/z)$ for all $n \geq 0$, $\nu \geq 0$,

it follows directly from the definition of $P_{n,\nu}(z)$ in (1.2) that

(3.25) $\frac{d^\nu}{dz^\nu} P^*_{n+\nu,0}(z) = \frac{(n+\nu)!}{n!} P^*_{n,\nu}(z)$ for all $n \geq 0$, $\nu \geq 0$.

Now, since $P^*_{n+\nu,0}(z)$ has, from (3.23), all its zeros in $|z| < ((n+\nu)\mu)^{-1}$, then, by the Gauss-Lucas Theorem (cf. Marden [5, p. 14]), the same is true for all derivatives of $P^*_{n+\nu,0}(z)$. In particular, from (3.25), $P^*_{n,\nu}(z)$ has all its zeros in $|z| < ((n+\nu)\mu)^{-1}$, which implies that $P_{n,\nu}(z)$ has all its zeros in $|z| > (n+\nu)\mu$, which gives the first inequality of (2.2) of Theorem 2.2.

Finally, the first inequality of (2.2) implies that

(3.26) $\mu \leq \inf_{\substack{n \geq 1 \\ \nu \geq 0}} \{\frac{|z|}{(n+\nu)} : P_{n,\nu}(z) = 0\}$.

To show that equality holds in (3.26), Szegö [13] has established that $\hat{z}$ is a limit point of zeros of $\{s_n(nz)\}_{n=1}^{\infty}$ iff $\hat{z}$ satisfies (1.1). As $\hat{z} = -\mu$ satisfies (1.1), then evidently equality holds in (3.26), completing the proof of Theorem 2.2. ∎

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