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Two-point Padé expansions for a family of analytic functions *

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Abstract: Each member $G(z)$ of a family of analytic functions defined by Stieltjes transforms is shown to be represented by a positive T-fraction, the approximants of which form the main diagonal in the two-point Padé table of $G(z)$. The positive T-fraction is shown to converge to $G(z)$ throughout a domain $D(a, b)=[z\colon z \notin [-b, -a]]$, uniformly on compact subsets. In addition, truncation error bounds are given for the approximants of the continued function; these bounds supplement previously known bounds and apply in part of the domain of $G(z)$ not covered by other bounds. The proofs of our results employ properties of orthogonal $\mathfrak{L}$-polynomials (Laurent polynomials) and $\mathfrak{L}$-Gaussian quadrature which are of some interest in themselves. A number of examples are considered.

Keywords: Padé approximant, continued fraction, $\mathfrak{L}$-Gaussian quadrature, orthogonal $\mathfrak{L}$-polynomials.

1. Introduction

For $0 \leqslant a < b \leqslant +\infty$, let $\Phi(a, b)$ denote the set of all bounded, nondecreasing functions $\phi(t)$, from $a < t < b$ into $\mathbb{R}$, which have infinitely many points of increase on (a, b) and for which the moments

$$c_k = \int_a^b (-t)^k \, \mathrm{d}\phi(t) \tag{1.1}$$

exist for all integer values of $k = 0, \pm 1, \pm 2, \ldots$ For $\phi(t) \in \Phi(a, b)$, the function $G(z)$ defined by the Riemann–Stieltjes integral

$$G(z) = z \int_a^b \frac{\mathrm{d}\phi(t)}{z+t} \tag{1.2}$$

is holomorphic in the cut plane $D(a, b) = [z\colon z \notin [-b, -a]]$. The series

$$L_0 = \sum_{n=1}^{\infty} -c_{-n} z^n, \qquad L_\infty = \sum_{n=0}^{\infty} c_n z^{-n} \tag{1.3}$$

are asymptotic expansions of $G(z)$ at $z = 0$ and $z = \infty$, respectively, with respect to the sector $R_\alpha = [z\colon |\mathrm{Arg}\, z| < \alpha]$, $0 < \alpha < \pi$ [21, Theorem 4.2]. The (n, n) two-point Padé approximant of (L_0, L_∞) (and of $G(z)$) is the nth approximant of the positive T-fraction

$$\frac{F_1 z}{1 + G_1 z} + \frac{F_2 z}{1 + G_2 z} + \frac{F_3 z}{1 + G_3 z} + \cdots, \quad F_m > 0, \; G_m > 0 \tag{1.4}$$

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corresponding to L_0 at $z = 0$ and to L_∞ at $z = \infty$.

The purpose of this paper is to investigate the positive T-fraction expansions of functions (1.2). It is shown (Theorem 2.1) that, if $b < +\infty$, then (1.4) converges to $G(z)$ for all $z \in D(a, b)$. In the discussion of truncation error bounds for the continued fractions (1.4), a new result is given (Theorem 3.2) for $z \notin [-b, -a]$, $z \in \mathbb{R}$. This complements the truncation error bounds already known for $z \in R = [z: |\text{Arg } z| < \pi]$ (see, for example, [9; 17, Theorem 2; 19, Theorem 8.11]. Examples dealt with in Section 4 include the complex exponential integral $E_1(w)$, the natural logarithm and Arctan w. A comparison, made between one-point and two-point Padé approximants of $E_1(w)$ for $w > 0$, points out advantages and disadvantages of each type of approximation. The convergence behavior of two-point Padé approximants of $E_1(w)$ for complex w is described by means of contour maps of the number of significant digits attained by various selected approximants. The paper also contains several results (Theorems 2.2–3.1) on orthogonal $\mathfrak{L}$-polynomials and $\mathfrak{L}$-Gaussian quadrature, which are used in the proofs of Theorem 2.1 and 3.2, and which are also of some interest in themselves.

Applications of two-point Padé approximants to theoretical physics have been made in a number of papers (see, for example, [1,16,26,27]). Many special functions represented by converging sequences of two-point Padé approximants (general T-fractions and the closely related M-fractions) can be found in [3,4,5,7,19,22,23,24,25,31]. Grundy [10,11,12] has applied M-fractions to Volterra integral equations and to inversion of Laplace transforms. Positive T-fractions have been used recently in the solution of the strong Stieltjes moment problem [21]. The computation of poles of two-point Padé approximants and positive T-fractions have been studied in [18]. Further results on two-point Padé approximants may be found in [9,17,30].

Before describing the results of this paper, we recall some pertinent facts about positive T-fractions (1.4) and about other continued fractions (real J-fractions and modified S-fractions) whose approximants lie in ordinary (one-point) Padé tables.

Let $\phi(t) \in \Phi(a, b)$ with $0 \leqslant a < b \leqslant +\infty$. Then the positive coefficients F_n and G_n in (1.4) are defined and can be calculated, in terms of the moments c_k in (1.1), by means of the FG-relations of McCabe and Murphy (see, for example, [24; 19, pp. 267–269]). To compute F_n, G_n for $n = 1, 2, \ldots, p$, first set

$$F_1^{(m)} = 0, \qquad G_1^{(m)} = -\frac{c_{-m-1}}{c_{-m}}, \quad m = -p, -p+1, \ldots, p-1. \tag{1.5a}$$

Then compute recursively, for $n = 1, 2, \ldots, p-1$

$$F_{n+1}^{(m)} = F_n^{(m+1)} + G_n^{(m+1)} - G_n^{(m)}, \quad m = n-p-1, n-p, \ldots, p-n-1, \tag{1.5b}$$

$$G_{n+1}^{(m)} = \frac{F_{n+1}^{(m)}}{F_{n+1}^{(m-1)}} G_n^{(m-1)}, \quad m = n-p, n-p+1, \ldots, p-n-1. \tag{1.5c}$$

Finally, set

$$F_1 = -c_{-1}, \qquad F_n = F_n^{(0)}, \quad n = 2, 3, \ldots, p, \tag{1.6a}$$

$$G_n = G_n^{(0)}, \quad n = 1, 2, \ldots, p. \tag{1.6b}$$

The resulting positive T-fraction (1.4) corresponds to L_0 at $z = 0$ and to L_∞ at $z = \infty$ in the sense that, if $f_n(z)$ denotes the nth approximant of (1.4), then

$$f_n(z) = -c_{-1}z - c_{-2}z^2 - \cdots - c_{-n}z^n + c_{-n-1}^{(n)}z^{n+1} + \cdots \tag{1.7a}$$

and

$$f_n(z) = c_0 + c_1 z^{-1} + \cdots + c_{n-1}z^{-n+1} + c_n^{(n)}z^{-n} + \cdots. \tag{1.7b}$$

Thus $f_n(z)$ is the (n, n) two-point Padé approximant of $G(z)$; similarly, it can be seen that the nth approximant of the closely related M-fraction

$$\frac{F_1}{1 + G_1 z} + \frac{F_2 z}{1 + G_2 z} + \frac{F_3 z}{1 + G_3 z} + \cdots$$

is the $(n-1, n)$ two-point Padé approximant of $z^{-1}G(z)$. If (1.4) converges at any point in the cut plane R_π, then it converges at every point in R_π, uniformly on compact subsets. A necessary and sufficient condition that (1.4) converges for $z \in R_\pi$ is that

$$\sum_{n=1}^{\infty} e_n = \infty \quad \text{or} \quad \sum_{n=1}^{\infty} d_n = \infty \tag{1.8a}$$

where the continued fraction

$$\frac{z}{e_1 + d_1 z} + \frac{z}{e_2 + d_2 z} + \frac{z}{e_3 + d_3 z} + \cdots, \quad e_n > 0,\ d_n > 0 \tag{1.8b}$$

is obtained from (1.4) by an equivalence transformation. We have

$$e_1 = 1/F_1, \qquad e_{2n-1} = \prod_{k=1}^{n-1} F_{2k} / \prod_{k=1}^{n} F_{2k-1}, \quad n = 2, 3, 4 \ldots, \tag{1.8c}$$

$$e_{2n} = 1/F_{2n} e_{2n-1}, \qquad d_n = G_n e_n, \quad n = 1, 2, 3, \ldots \tag{1.8d}$$

[21, pp. 508–509 and Theorem 2.2]. A sufficient condition for convergence of (1.4) for all $z \in R_\pi$ is that [9]

$$\sum_{n=2}^{\infty} |c_n c_{-n}|^{-1/4(n-1)} = \infty. \tag{1.9}$$

We turn now briefly to real J-fractions and modified S-fractions. For that purpose we consider $-\infty \leqslant a < b \leqslant +\infty$ and let $\Phi^c(a, b)$ denote the set of all bounded, nondecreasing functions $\phi(t)$, from $a < t < b$ into $\mathbb{R}$, which have infinitely many points of increase on (a, b) and for which the moments (1.1) exist for the non-negative integers $k = 0, 1, 2, \ldots$. The right side of (1.2) defines a function $G^+(z)$ holomorphic for $z \in R^+ = [z\colon \operatorname{Im} z > 0]$ and a function $G^-(z)$ holomorphic for $z \in R^- = [z\colon \operatorname{Im} z < 0]$. The series L_∞ in (1.3) is the asymptotic expansion of $G^+(z)$ $(G^-(z))$ at $z = \infty$ with respect to R^+ (R^-). There exists a real J-fraction

$$\frac{k_1 z}{l_1 + z} - \frac{k_2}{l_2 + z} - \frac{k_3}{l_3 + z} - \cdots, \quad k_n > 0, \quad l_n \in \mathbb{R}, \tag{1.10}$$

which corresponds to L_∞ at $z = \infty$ in the sense that, if $J_n(z)$ denotes the nth approximant of (1.10), then

$$J_n(z) = c_0 + c_1 z^{-1} + \cdots + c_{2n-1} z^{-2n+1} + \lambda_{2n}^{(n)} z^{-2n} + \cdots. \tag{1.11}$$

Thus $J_n(z)$ is the $(n-1, n)$ Padé approximant of L_∞ at $z = \infty$. The coefficients k_n, l_n may be computed by an algorithm described in [8; 19, Algorithm 7.2.1]. In the special case in which $[a, b]$ is a finite interval, Markoff's theorem asserts that (1.10) converges to (1.2) for all $z \in D(a, b)$. Thus Theorem 2.1 is the analogue of Markoff's theorem for positive T-fractions.

Considerably more can be said about the continued fraction representation of (1.2) when $\phi(t) \in \Phi^c(a, b)$ with $0 \leqslant a < b \leqslant +\infty$. In that case the function $G(z)$ in (1.2) is holomorphic in the cut plane R_π and L_∞ is the asymptotic expansion of $G(z)$ at $z = \infty$ with respect to the sectors R_α, $0 < \alpha < \pi$. There exists a modified S-fraction

$$\frac{c_0}{1} - \frac{q_1^{(0)}}{z} - \frac{e_1^{(0)}}{1} - \frac{q_2^{(0)}}{z} - \frac{e_2^{(0)}}{z} - \cdots, \quad q_n^{(0)} < 0,\ e_n^{(0)} < 0 \tag{1.12}$$

which corresponds to L_∞ in (1.3) at $z = \infty$ in the sense that, if $h_n(z)$ denotes the nth approximant of (1.12), then

$$h_n(z) = c_0 + c_1 z^{-1} + \cdots + c_{n-1} z^{-n+1} + \mu_n^{(n)} z^{-n} + \cdots. \tag{1.13}$$

Thus $h_{2m}(z)$ $(h_{2m+1}(z))$ is the $(m-1, m)$ $((m, m))$ Padé approximant of L_∞ at $z = \infty$. The coefficients $q_n^{(0)}$, $e_n^{(0)}$ may be computed by means of the qd-relations (see, for example, [13, p. 609; p. 227]). If (1.12) converges for one $z \in R_\pi$, then it converges to (1.2) for all $z \in R_\pi$. A necessary and sufficient condition for convergence of (1.12) for $z \in R_\pi$ is that

$$\sum_{n=1}^{\infty} b_n = \infty \tag{1.14}$$

where

$$\frac{1}{b_1} + \frac{1}{b_2 z} + \frac{1}{b_3} + \frac{1}{b_4 z} + \cdots$$

is obtained from (1.12) by an equivalence transformation. Carleman's condition $\sum_1^\infty c_n^{-1/2n} = \infty$ is sufficient for the convergence of (1.12). The even part of (1.10) is the real J-fraction

$$\frac{c_0 z}{z - q_1^{(0)}} - \frac{q_1^{(0)} e_1^{(0)}}{z - \left(e_1^{(0)} + q_2^{(0)}\right)} - \frac{q_2^{(0)} e_2^{(0)}}{z - \left(e_2^{(0)} + q_3^{(0)}\right)} - \cdots; \tag{1.15}$$

it converges to (1.2) for all $z \in D(a, b)$, provided $0 \leqslant a < b < +\infty$.

2. Positive T-fraction expansions

The main result of this section is the following.

Theorem 2.1. *Let $\phi(t) \in \Phi(a, b)$ with $0 \leqslant a < b < +\infty$. Then for all $z \in D(a, b) = [z: z \notin [-b, -a]]$,*

$$G(z) = z\int_a^b \frac{d\phi(t)}{z+t} = \frac{F_1 z}{1 + G_1 z} + \frac{F_2 z}{1 + G_2 z} + \frac{F_3 z}{1 + G_3 z} + \cdots, \tag{2.1}$$

where the positive coefficients F_n, G_n are given by (1.5) *and* (1.6). *The positive T-fraction converges uniformly on every compact subset of $D(a, b)$ to the holomorphic function $G(z)$.*

Before proving the theorem, we shall describe some results on orthogonal $\mathfrak{L}$-polynomials and $\mathfrak{L}$-Gaussian quadrature that will subsequently be used. A brief sketch of some of these proofs is included in [20].

A function $R(z)$ of the form

$$R(z) = \sum_{j=k}^{m} r_j z^j, \quad r_j \in \mathbb{R}, \quad -\infty < k \leqslant m < +\infty$$

is called an *$\mathfrak{L}$-polynomial* (or *Laurent polynomial*) in the complex variable z. The set $\mathfrak{R}$ of all $\mathfrak{L}$-polynomials forms a linear space over $\mathbb{R}$ with respect to the usual definitions of addition and scalar multiplication. A basis for $\mathfrak{R}$ is given by $1, z^{-1}, z, z^{-2}, z^2, \ldots$. For $m \geqslant 0$, we let $\mathfrak{R}_{2m}$ and $\mathfrak{R}_{2m+1}$ denote the subspaces spanned by $z^{-m}, z^{-m+1}, \ldots, z^m$ and $z^{-m-1}, z^{-m}, \ldots, z^m$, respectively. If $\phi(t) \in \Phi(a, b)$ with $0 \leqslant a < b \leqslant +\infty$, then

$$(R, S) = \int_a^b R(t) S(t) d\phi(t), \quad R, S \in \mathfrak{R}$$

defines an inner product on $\mathfrak{R}$. In fact, linearity, symmetry and homogeneity follow directly from properties of the Riemann–Stieltjes integral. To prove positivity we note that

$$(R, R) = \int_a^b [R(t)]^2 d\phi(t) \geqslant 0 \quad \text{for all } R \in \mathfrak{R}$$

and, since ϕ has infinitely many points of increase on (a, b), $(R, R) = 0$ if and only if $R(t) \equiv 0$. The norm $\|R\|$ of R is defined by $\|R\| = (R, R)^{1/2}$.

We recall that the Hankel determinants $H_k^{(m)}$, associated with a double sequence $\{c_n\}_{-\infty}^{\infty}$, are defined by

$H_k^{(m)}=1$ if $k \leqslant 0$ and

$$H_k^{(m)}=\begin{vmatrix} c_m & c_{m+1} & \cdots & c_{m+k-1} \\ c_{m+1} & c_{m+2} & \cdots & c_{m+k} \\ \vdots & \vdots & & \vdots \\ c_{m+k-1} & c_{m+k} & \cdots & c_{m+2k-2} \end{vmatrix}, \quad k=1,2,3,\ldots,\quad m=0,\pm 1,\pm 2,\cdots$$

Corresponding to each $\phi(t) \in \Phi(a, b)$ with $0 \leqslant a < b \leqslant +\infty$, we shall consider the sequence of $\mathfrak{L}$-polynomials $\{Q_n(z)\}_0^\infty$ defined by $Q_0(z)=1$,

$$Q_{2n}(z)=\frac{(-1)^n}{H_{2n}^{(-2n+1)}}\begin{vmatrix} c_{-2n} & \cdots & c_{-1} & (-z)^{-n} \\ \vdots & & \vdots & \vdots \\ c_{-1} & \cdots & c_{2n-2} & (-z)^{n-1} \\ c_0 & \cdots & c_{2n-1} & (-z)^n \end{vmatrix}, \quad n=1,2,3,\ldots, \tag{2.2a}$$

$$Q_{2n+1}(z)=\frac{(-1)^n}{H_{2n+1}^{(-2n)}}\begin{vmatrix} c_{-2n-1} & \cdots & c_{-1} & (-z)^{-n-1} \\ \vdots & & \vdots & \vdots \\ c_{-2} & \cdots & c_{2n-1} & (-z)^{n-1} \\ c_0 & \cdots & c_{2n} & (-z)^n \end{vmatrix}, \quad n=0,1,2,\ldots \tag{2.2b}$$

In the sequel we shall write

$$Q_{2n}(z)=\sum_{j=-n}^{n} q_{2n,j}z^j, \qquad Q_{2n+1}(z)=\sum_{j=-n-1}^{n} q_{2n+1,j}z^j, \quad n=0,1,2,\ldots \tag{2.3}$$

Clearly $Q_n(z) \in \mathfrak{R}_n$.

Theorem 2.2. *Let* $\phi(t) \in \Phi(a, b)$ *with* $0 \leqslant a < b \leqslant +\infty$ *and let* $\{Q_n(z)\}_{n=0}^\infty$ *be defined by* (2.2). *Then*:

(A) *Orthogonality and normalization:*

$$(Q_n, Q_m)=\begin{cases} 0, & \text{if } n \neq m, \\ \|Q_n\|^2 > 0, & \text{if } n=m, \end{cases} \tag{2.4}$$

$$\|Q_{2n}\|^2=\frac{H_{2n}^{(-2n)}H_{2n+1}^{(-2n)}}{\left[H_{2n}^{(-2n+1)}\right]^2}, \qquad \|Q_{2n+1}\|^2=\frac{H_{2n+2}^{(-2n-2)}}{H_{2n+1}^{(-2n)}}, \quad n=0,1,2,\ldots, \tag{2.5}$$

$$q_{2n,-n}=q_{2n+1,-n-1}=1, \qquad q_{2n,n}=\frac{H_{2n}^{(-2n)}}{H_{2n}^{(-2n+1)}}>0, \qquad q_{2n+1,n}=\frac{H_{2n+1}^{(-2n-1)}}{H_{2n+1}^{(-2n)}}<0, \tag{2.6}$$

$n=0,1,2,\ldots$

(B) *Three-term recurrence relations*:

$$Q_0(z)=1, \qquad Q_1(z)=z^{-1}+q_{1,0}, \tag{2.7a}$$

and for $n=1,2,3,\ldots$

$$Q_{2n}(z)=(1-G_{2n}z)Q_{2n-1}(z)-F_{2n}Q_{2n-2}(z), \tag{2.7b}$$

$$Q_{2n+1}(z)=\left(z^{-1}-G_{2n+1}\right)Q_{2n}(z)-F_{2n+1}Q_{2n-1}(z), \tag{2.7c}$$

where the F_n *and* G_n *are defined by* (1.5) *and* (1.6).

(C) *Continued fraction*: *If $B_n(z)$ denotes the nth denomimator of the positive T-fraction* (1.4), *then*

$$Q_{2n}(z)=B_{2n}(-z)/z^n, \qquad Q_{2n+1}(z)=B_{2n+1}(-z)/z^{n+1}, \quad n=0,1,2,\ldots \tag{2.8}$$

(D) *Zeros*: *For each $n=1,2,3,\ldots$, $Q_n(z)$ has exactly n zeros $t_1^{(n)}, t_2^{(n)},\ldots,t_n^{(n)}$. They are distinct, positive, real numbers and all lie in (a, b).*

Proof. (A) Using (2.2) and the known fact that $H_n^{(-n+1)}>0$, $H_{2n}^{(-2n)}>0$ and $H_{2n-1}^{(-2n+1)}<0$ for $n\geqslant 1$ [21, Theorem 9.8C], one can readily show that, for $n=0,1,2,\ldots,$

$$(z^k, Q_{2n})=0, \quad -n\leqslant k\leqslant n-1,$$

$$\|Q_{2n}\|^2=(Q_{2n},Q_{2n})=q_{2n,n}(z^n,Q_{2n})=\frac{H_{2n}^{(-2n)}H_{2n+1}^{(-2n)}}{\left[H_{2n}^{(-2n+1)}\right]^2}>0,$$

$$(z^k, Q_{2n+1})=0, \quad -n\leqslant k\leqslant n,$$

$$\|Q_{2k+1}\|^2=(Q_{2k+1},Q_{2k+1})=(z^{-n-1},Q_{2n+1})=\frac{H_{2n+2}^{(-2n-2)}}{H_{2n+1}^{(-2n)}}>0.$$

From this we obtain (2.4) and (2.5). (2.6) is easily verified from (2.2).

(B) can be verified by using (2.14) and an argument that is standard for orthogonal polynomials.

(C) follows by comparing (2.7) with the difference equations satisfied by the denominators $B_n(z)$ of the continued fraction (1.4).

(D) We shall show that $Q_{2n}(z)$ has $2n$ zeros and that they are real, distinct and lie in (a, b). The proof for $Q_{2n+1}(z)$ is completely analogous and hence is omitted. Let λ denote the number of distinct real zeros of $Q_{2n}(z)$ that lie in (a, b). We denote these by $t_1, t_2,\ldots,t_\lambda$ and consider

$$I_{2n}=\int_a^b Q_{2n}(t)\left[\prod_{j=1}^{\lambda}(1-t/t_j)/t^n\right]\mathrm{d}\phi(t)=\int_a^b S_{2n}(t)\left[\prod_{j=1}^{\lambda}(1-t/t_j)^2 t^{2n}\right]\mathrm{d}\phi(t)$$

where $S_{2n}(t)$ is a polynomial in t that does not change sign on $[a, b]$ and is not identically zero. Since $\phi(t)$ is assumed to have infinitely many points of increase on (a, b), it follows that $I_{2n}\neq 0$. On the other hand I_{2n} can be written in the form

$$I_{2n}=\int_a^b Q_{2n}(t)\left[t^{-n}+d_{-n+1}t^{-n+1}+\cdots+d_{\lambda-n}t^{\lambda-n}\right]\mathrm{d}\phi(t).$$

Therefore by orthogonality we would have $I_{2n}=0$ if $\lambda\leqslant 2n-1$. Thus $\lambda=2n$, which proves (D). □

Theorem 2.3 ($\mathfrak{L}$-*Gaussian quadrature*). *Let $\phi(t)\in\Phi(a, b)$ with $0\leqslant a<b\leqslant+\infty$. Let $t_1^{(n)}, t_2^{(n)},\ldots,t_n^{(n)}$ denote the n zeros of the orthogonal $\mathfrak{L}$-polynomial $Q_n(z)$. Then for every $F(z)\in\mathbb{R}_{2n-1}$,*

$$\int_a^b F(t)\mathrm{d}\phi(t)=\sum_{j=1}^{n} w_j^{(n)}F\left(t_j^{(n)}\right), \tag{2.9}$$

where

$$w_j^{(n)}=\frac{1}{Q_n'\left(t_j^{(n)}\right)}\int_a^b\frac{Q_n(t)}{t-t_j^{(n)}}\mathrm{d}\phi(t), \quad j=1,2,\ldots,n. \tag{2.10}$$

Proof. Let $F(z)\in\mathfrak{R}_{2n-1}$ be given and let

$$L_{n,j}(z)=\frac{Q_n(z)}{\left(z-t_j^{(n)}\right)Q_n'\left(t_j^{(n)}\right)}, \quad j=1,2,\ldots,n. \tag{2.11}$$

It is readily seen that $L_{n,j}(z) \in \mathfrak{R}_{2n-1}$ and that $L_{n,k}(t_j^{(n)}) = \delta_{k,j}$ (the Kronecker delta). Let

$$R(z) = \sum_{k=1}^{n} L_{n,k}(z) F(t_k^{(n)}).$$

Then $R(z) \in \mathfrak{R}_{n-1}$ and $R(t_j^{(n)}) = F(t_j^{(n)})$, $j = 1, 2, \ldots, n$. Therefore $F(z) - R(z) \in \mathfrak{R}_{2n-1}$ and zeros at $t_1^{(n)}$, $t_2^{(n)}, \ldots, t_n^{(n)}$. It then follows that

$$S(z) = [F(z) - R(z)]/Q_n(z) \in \mathfrak{R}_{n-1}.$$

Hence

$$\int_a^b F(t)\mathrm{d}\phi(t) = \int_a^b R(t)\mathrm{d}\phi(t) + \int_a^b Q_n(t)S(t)\mathrm{d}\phi(t).$$

The second integral on the right vanishes by orthogonality, and we obtain

$$\int_a^b F(t)\mathrm{d}\phi(t) = \sum_{j=1}^{n} F(t_j^{(n)}) \int_a^b L_{n,j}(t)\mathrm{d}\phi(t) = \sum_{j=1}^{n} w_j^{(n)} F(t_j^{(n)}). \qquad \square$$

The numbers $t_j^{(n)}$ and $w_j^{(n)}$ in Theorem 2.3 are called, respectively, the *abscissae* and *weights* of the n-point $\mathfrak{L}$-Gaussian quadrature formula (2.9). Some applications of $\mathfrak{L}$-Gaussian quadrature to the numerical evaluation of integrals are described in [20]. For an interesting recent survey of classical Gaussian quadrature see [6].

Theorem 2.4. *Let $\phi(t) \in \Phi(a, b)$ with $0 \leqslant a < b < +\infty$. Let $t_j^{(n)}$ and $w_j^{(n)}$, $j = 1, 2, \ldots, n$, denote the abscissae and weights of the n-point $\mathfrak{L}$-Gaussian quadrature formula with respect to $\phi(t)$. Let $F(t)$ be a function of the form*

$$F(t) = f(t)/t^m$$

where m is a fixed integer and $f(t)$ is a bounded, Riemann–Stieltjes integrable function with respect to $\phi(t)$ on $[a, b]$. Then

$$\int_a^b F(t)\mathrm{d}\phi(t) = \lim_{n\to\infty} \sum_{j=1}^{n} w_j^{(n)} F(t_j^{(n)}). \tag{2.12}$$

Proof. We first note that the integral on the left side of (2.12) may be an improper Riemann–Stieltjes integral. Let $\epsilon > 0$ be given. From [28, Theorem, 1.5.4] there exist polynomials p and q such that

$$-M - \epsilon < p(t) \leqslant f(t) \leqslant q(t) \leqslant M + \epsilon, \quad \text{for } a \leqslant t \leqslant b, \tag{2.13}$$

where

$$M = \max\left\{\left|\sup_{a\leqslant t\leqslant b} f(t)\right|, \left|\inf_{a\leqslant t\leqslant b} f(t)\right|\right\} \quad \text{and} \quad \int_a^b [q(t) - p(t)]\mathrm{d}\phi(t) < \epsilon.$$

We observe that

$$\int_a^b [q(t) - p(t)]^2 \mathrm{d}\phi(t) \leqslant \int_a^b 2(M+\epsilon)[q(t) - p(t)]\mathrm{d}\phi(t) \leqslant 2\epsilon(M+\epsilon).$$

Now define $P(t) = p(t)/t^m$ and $Q(t) = q(t)/t^m$. Then $P(t)$ and $Q(t)$ are $\mathfrak{L}$-polynomials and by (2.13)

$$P(t) \leqslant F(t) \leqslant Q(t), \quad \text{for } t \neq 0. \tag{2.14}$$

By Theorem 2.3 there exists an integer n_0 such that, for all $n \geqslant n_0$, the quadrature formula with n points is exact for P and Q; that is,

$$\int_a^b P(t)\mathrm{d}\phi(t) = \sum_{j=1}^{n} w_j^{(n)} P(t_j^{(n)}), \qquad \int_a^b Q(t)\mathrm{d}\phi(t) = \sum_{j=1}^{n} w_j^{(n)} Q(t_j^{(n)}), \quad n \geqslant n_0.$$

Consequently,

$$\begin{aligned}\sum_{j=1}^{n} w_j^{(n)} Q\left(t_j^{(n)}\right) - \sum_{j=1}^{n} w_j^{(n)} P\left(t_j^{(n)}\right) &= \int_a^b [Q(t) - P(t)] \mathrm{d}\phi(t) \\ &= \int_a^b \frac{q(t) - p(t)}{t^m} \mathrm{d}\phi(t) \\ &\leqslant \left[\int_a^b [q(t) - p(t)]^2 \mathrm{d}\phi(t)\right]^{1/2} \left[\int_a^b t^{-2m} \mathrm{d}\phi(t)\right]^{1/2} \\ &\leqslant \sqrt{2\epsilon(M+\epsilon) c_{-2m}}\end{aligned}$$

where $c_{-2m} = \int_a^b t^{-2m} \mathrm{d}\phi(t)$. The first inequality above follows from Schwarz' inequality. By (2.14) we then have

$$\begin{aligned}\sum_{j=1}^{n} w_j^{(n)} Q\left(t_j^{(n)}\right) - \sum_{j=1}^{n} w_j^{(n)} F\left(t_j^{(n)}\right) &\leqslant \sum_{j=1}^{n} w_j^{(n)} Q\left(t_j^{(n)}\right) - \sum_{j=1}^{n} w_j^{(n)} F\left(t_j^{(n)}\right) \\ &\leqslant \sqrt{2\epsilon(M+\epsilon) c_{-2m}}.\end{aligned}$$

Hence for all $n \geqslant n_0$.

$$\begin{aligned}&\left|\int_a^b F(t) \mathrm{d}\phi(t) - \sum_{j=1}^{n} w_j^{(n)} F\left(t_j^{(n)}\right)\right| \\ &\quad\leqslant \left|\int_a^b F(t) \mathrm{d}\phi(t) - \int_a^b Q(t) \mathrm{d}\phi(t)\right| + \left|\int_a^b Q(t) \mathrm{d}\phi(t) - \sum_{j=1}^{n} w_j^{(n)} F\left(t_j^{(n)}\right)\right| \\ &\quad\leqslant \int_a^b [Q(t) - P(t)] \mathrm{d}\phi(t) + \sum_{j=1}^{n} w_j^{(n)} \left[Q\left(t_j^{(n)}\right) - F\left(t_j^{(n)}\right)\right] \\ &\quad\leqslant 2\sqrt{2\epsilon(M+\epsilon) c_{-2m}}. \qquad \square\end{aligned}$$

Proof of Theorem 2.1. Let $A_n(z)$ and $B_n(z)$ denote the nth denominator, respectively, of the positive T-fraction in (1.4). We shall establish the partial fraction decomposition

$$\frac{A_n(z)}{B_n(z)} = \sum_{j=1}^{n} \frac{z w_j^{(n)}}{z + t_j^{(n)}}, \tag{2.15}$$

and the relations

$$\sum_{j=1}^{n} w_j^{(n)} = \frac{F_1}{G_1}, \quad w_j^{(n)} > 0,\ j = 1, 2, \ldots, n. \tag{2.16}$$

It was shown in [21, pp. 513–514] that $A_n(z)/B_n(z)$ can be expressed in the form

$$\frac{A_n(z)}{B_n(z)} = \sum_{j=1}^{n} \frac{z \pi_j^{(n)}}{z + t_j^{(n)}} \tag{2.17}$$

where

$$\sum_{j=1}^{n} \pi_j^{(n)} = \frac{F_1}{G_1}, \quad \pi_j^{(n)} > 0,\ j = 1, 2, \ldots, n.$$

If suffices then to show that $\pi_j^{(n)} = w_j^{(n)}$. For that purpose we consider the sequence of $\mathfrak{L}$-polynomials

$\{P_n(z)\}_0^\infty$ defined by

$$P_0(z)=1, \qquad P_1(z)=-F_1, \tag{2.18a}$$

$$P_{2n}(z)=(1-G_{2n}z)P_{2n-1}(z)-F_{2n}P_{2n-2}(z), \quad n=1,2,3,\ldots, \tag{2.18b}$$

$$P_{2n+1}(z)=(z^{-1}-G_{2n+1})P_{2n}(z)-F_{2n+1}P_{2n-1}(z), \quad n=1,2,3,\ldots \tag{2.18c}$$

By comparing (2.18) with the difference equations satisfied by the $A_n(z)$, we see that

$$P_{2n}(z)=A_{2n}(-z)/z^n, \qquad P_{2n+1}(z)=A_{2n+1}(-z)/z^{n+1}, \quad n=0,1,2,\ldots$$

Therefore

$$\frac{P_n(z)}{Q_n(z)}=\frac{A_n(-z)}{B_n(-z)}=\sum_{j=1}^{n}\frac{z\pi_j^{(n)}}{z-t_j^{(n)}},$$

and hence

$$\pi_j^{(n)}=\lim_{z\to t_j^{(n)}}\frac{\left(z-t_j^{(n)}\right)P_n(z)}{zQ_n(z)}=\frac{P_n\left(t_j^{(n)}\right)}{t_j^{(n)}Q_n'\left(t_j^{(n)}\right)}, \quad j=1,2,\ldots,n. \tag{2.19}$$

It can also be shown that

$$P_n(z)=z\int_a^b\frac{Q_n(z)-Q_n(t)}{z-t}\,\mathrm{d}\phi(t), \quad n=0,1,2,\ldots \tag{2.20}$$

In fact, let $\hat{P}_n(z)$ denote the right side of (2.20). Then by induction, using orthogonality of the $Q_n(t)$ and (2.7), one can show that the $\hat{P}_n(z)$ satisfy the recurrence relations (2.18). Hence $\hat{P}_n(z)=P_n(z)$, $n=0, 1, 2, \ldots$. From (2.20) we obtain

$$P_n\left(t_j^{(n)}\right)=t_j^{(n)}\int_a^b\frac{Q_n(t)}{t-t_j^{(n)}}\,\mathrm{d}\phi(t), \quad j=1,2,\ldots,n.$$

Combining this with (2.10) and (2.19) yields

$$w_j^{(n)}=\frac{P_n\left(t_j^{(n)}\right)}{t_j^{(n)}Q_n'\left(t_j^{(n)}\right)}=\pi_j^{(n)}, \quad j=1,2,\ldots,n.$$

Now, for fixed $z\in D(a,b)$, set $F(t)=z/(z+t)$. Then by (2.15) and Theorem 2.4,

$$z\int_a^b\frac{\mathrm{d}\phi(t)}{z+t}=\lim_{n\to\infty}\sum_{j=1}^{n}\frac{zw_j^{(n)}}{z+t_j^{(n)}}=\lim\frac{A_n(z)}{B_n(z)},$$

which proves the convergence of (2.1). Let K be an arbitrary compact subset of $D(a,b)$. Then there exist constants $B(K)$ and $\delta(K)$ such that, for all $z\in K$, we have $|z|\leqslant B(K)$ and $|z+t_j^{(k)}|\geqslant\delta(K)$, $j=1,2,\ldots,n$, $n=1, 2, 3, \ldots$. Therefore

$$\left|\frac{A_n(z)}{B_n(z)}\right|\leqslant\sum_{j=1}^{n}\frac{|z|w_j^{(n)}}{|z+t_j^{(n)}|}\leqslant\frac{F_1B(K)}{G_1\delta(K)}, \quad z\in K, \quad n=1,2,3,\ldots$$

It follows that $\{A_n(z)/B_n(z)\}$ is a normal family of holomorphic functions in $D(a,b)$ and hence by the Stieltjes–Vitali theorem ([15, Theorem 15.3.1; 29, Theorem 20.15 and Remark 20.2]), the sequence $\{A_n(z)/B_n(z)\}$ converges uniformly on K. □

3. Truncation error estimates

For positive T-fractions (1.4) the following a posteriori truncation error bounds are known. If $f_n(z) = A_n(z)/B_n(z)$ denotes the nth approximant of (1.4), then for $n = 2, 3, 4, \ldots$ and $m = 0, 1, 2, \ldots$,

$$|f_{n+m}(z) - f_n(z)| \leqslant K(z)|f_n(z) - f_{n-1}(z)| \tag{3.1a}$$

where

$$K(z) = \begin{cases} 1, & \text{if } 0 \leqslant |\arg z| \leqslant \frac{1}{2}\pi, \\ \csc|\arg z|, & \text{if } \frac{1}{2}\pi < |\arg z| < \pi, \end{cases} \tag{3.1b}$$

(see, for example, [9; 17, Theorem 2; 19, Theorem 8.11]). If the continued fraction (1.4) converges to a function $G(z)$ (as in Theorem 2.1), then $f_{n+m}(z)$ in (3.1a) may be replaced by $G(z)$. A priori truncation error bounds for (1.4) are also included in [9] for the same values of z. A limitation of (3.1) is that it tells nothing about the truncation error when z is real and negative; in particular, for $z \notin [-b, -a]$, $z \in \mathbb{R}$ at which points the continued fraction of Theorem 2.1 is convergent. This problem can be resolved to some extent by finding truncation error bounds for $\mathfrak{L}$-Gaussian quadrature since, by (2.15), the nth approximant $A_n(z)/B_n(z)$ of (2.1) is exactly equal to the n-point $\mathfrak{L}$-Gaussian quadrature approximation of the integral in (2.1). Such truncation error bounds are given in Theorems 3.1 and 3.2. Before stating and proving those results, we shall give some additional properties of orthogonal $\mathfrak{L}$-polynomials that are used.

We consider now the sequence of orthonormal $\mathfrak{L}$-polynomials $\{R_n^*(z)\}_{n=0}^{\infty}$ defined by

$$R_{2n}^*(z) = Q_{2n}(z)/\|Q_{2n}\|, \qquad R_{2n+1}^*(z) = -Q_{2n+1}(z)/\|Q_{2n+1}\|.$$

Clearly $(R_n^*, R_m^*) = \delta_{n,m}$. If the $R_n^*(z)$ are written in the form

$$R_{2n}^*(z) = k_{2n}\left(z - t_1^{(2n)}\right) \cdots \left(z - t_{2n}^{(2n)}\right)/z^n, \tag{3.2a}$$

$$R_{2n+1}^*(z) = k_{2n+1}\left(z - t_1^{(2n+1)}\right) \cdots \left(z - t_{2n+1}^{(2n+1)}\right)/z^{n+1}, \tag{3.2b}$$

then it is easily seen that, for $n = 0, 1, 2, \ldots$,

$$k_{2n} = q_{2n,n}/\|Q_{2n}\| \quad \text{and} \quad k_{2n+1} = -q_{2n+1,n}/\|Q_{2n+1}\|. \tag{3.2c}$$

It can be shown that, for $n = 0, 1, 2, \ldots$,

$$q_{2n,n} = \prod_{k=1}^{2n} G_k, \qquad q_{2n+1,n} = -\prod_{k=1}^{2n+1} G_k \tag{3.3}$$

and

$$\|Q_{2n}\|^2 = \prod_{k=1}^{2n+1} F_k/G_{2n+1}, \qquad \|Q_{2n+1}\|^2 = \prod_{k=1}^{2n+2} F_k. \tag{3.4}$$

The latter equations can be proved by induction, using (2.5) and the relations

$$H_1^{(-1)} = -F_1, \qquad H_n^{(-n)} = (-1)^n \prod_{k=1}^{n} F_k \prod_{k=1}^{n-1} u_k, \quad n = 2, 3, 4, \ldots,$$

$$H_n^{(-n+1)} = \prod_{k=1}^{n} u_k, \quad n = 1, 2, 3, \ldots,$$

where $u_k = \prod_{j=1}^{k}(F_j/G_j)$. Substituting (3.3) and (3.4) in (3.2), we arrive at the relations $k_0^2 = G_1/F_1$ and

$$k_{2n}^2 = \prod_{k=1}^{2n} G_k \prod_{k=1}^{2n+1} (G_k/F_k) = k_{2n-1}^2 G_{2n}^2 (G_{2n+1}/F_{2n+1}), \quad n = 1, 2, 3, \ldots, \tag{3.5a}$$

$$k_{2n+1}^2 = \prod_{k=1}^{2n+1} G_k \prod_{k=1}^{2n+1} (G_k/F_k)/F_{2n+2} = k_{2n}^2 (G_{2n+1}/F_{2n+2}), \quad n = 0, 1, 2, \ldots \tag{3.5b}$$

These can be used to compute the k_n in terms of the coefficients F_n and G_n.

Theorem 3.1. *Let $\phi(t) \in \Phi(a, b)$ with $0 \leqslant a < b < +\infty$ and let $t_j^{(n)}$ and $w_j^{(n)}$ denote the abscissae and weights for the n-point $\mathfrak{L}$-Gaussian quadrature with respect to $\phi(t)$. Let $f(t)$ be a real valued function for which $f^{(2n)}(t)$ exists for $a \leqslant t \leqslant b$ and let $F(t) = f(t)/t^n$. Then*

$$\int_a^b F(t)\,\mathrm{d}\phi(t) = \sum_{j=1}^{n} w_j^{(n)} F\left(t_j^{(n)}\right) + e_n(F) \tag{3.6}$$

where

$$\begin{aligned} e_n(F) &= \frac{\delta(n) f^{(2n)}(\eta)}{k_n^2 (2n)!}, \\ a < \eta < b, \quad \delta(n) &= \begin{cases} 1, & \text{if } n \text{ even}, \\ b, & \text{if } n \text{ odd}. \end{cases} \end{aligned} \tag{3.7}$$

We shall merely sketch the proof of Theorem 3.1 since it parallels rather closely the proof for the analogous theorem for Gaussian quadrature (see, for example, [14, pp. 314–323; 2, Theorem 14.2.2]).

Sketch of Proof. Let $t_1, \ldots, t_n$ be distinct numbers in (a, b) and

$$\Lambda_{n,k}(t) = t_k^{m(n)} \prod_{\substack{j=1 \\ j \neq k}}^{n} (t - t_j) / t^{m(n)} \prod_{\substack{j=1 \\ j \neq k}}^{n} (t_k - t_j), \quad k = 1, 2, \ldots, n$$

where $m(n) = \frac{1}{2}n$ if n is even and $m(n) = \frac{1}{2}(n-1)$ if n is odd. Then $\Lambda_{n,k} \in \mathfrak{R}_{n-1}$, $\Lambda_{n,k}^2 \in \mathfrak{R}_{2n-1}$ and $\Lambda_{n,k}(t_j) = \delta_{k,j}$. For $k = 1, \ldots, n$, let

$$\begin{aligned} S_{n,k}(t) &= \left[1 - 2\alpha_{n,k}(t)(t - t_k)\Lambda'_{n,k}(t_k)\right]\Lambda_{n,k}^2(t), \\ T_{n,k}(t) &= \alpha_{n,k}(t)(t - t_k)\Lambda_{n,k}^2(t) \end{aligned} \tag{3.8}$$

where $\alpha_{n,k}(t) = 1$ for n even and $\alpha_{n,k}(t) = t_k/t$ for n odd. Then $S_{n,k}(t), T_{n,k}(t) \in \mathfrak{R}_{2n-1}$, $S_{n,k}(t_j) = T'_{n,k}(t_j) = \delta_{k,j}$ and $S'_{n,k}(t_j) = T_{n,k}(t_j) = 0$ for $j, k = 1, \ldots, n$. Now let

$$H_n(t) = \sum_{k=1}^{n} F_k S_{n,k}(t) + \sum_{k=1}^{n} F'_k T_{n,k}(t) \tag{3.9}$$

where $F_k = F(t_k)$ and $F'_k = F'(t_k)$. Then $H_n(t) \in \mathfrak{R}_{2n-1}$, $H_n(t_j) = F_j$ and $H'_n(t_j) = F'_j$ for $j = 1, \ldots, n$. Moreover, $H_n(t)$ is the unique element of $\mathfrak{R}_{2n-1}$ satisfying these properties. $H_n(t)$ is called the *Hermite interpolating $\mathfrak{L}$-polynomial for $F(t)$ at $t_1, \ldots, t_n$.*

We now show that, for each $x \in (a, b)$, there exists $\xi = \xi(x)$ in (a, b) such that

$$f(x) = H_n(x) + f^{(2n)}(\xi) u(x) / (2n)! x^n \quad \text{where} \quad u(x) = \prod_{j=1}^{n} (t - t_j)^2. \tag{3.10}$$

We assume that $x \notin [t_1, \ldots, t_n]$ since otherwise (3.10) holds. Let

$$V(t) = \left[F(t) - H_n(t)\right] t^n - K(x) u(t) \quad \text{where} \quad K(x) = \left[F(x) - H_n(x)\right] x^n / u(x). \tag{3.11}$$

Then $V(t)$ vanishes at $x, t_1, \ldots, t_n$. Since $t^n H_n(t)$ is a polynomial and $f(t) = t^n F(t)$, $V^{(2n)}(t)$ exists in (a, b). Hence by Rolle's theorem $V'(t)$ has n distinct zeros in (a, b) but not in $[x, t_1, \ldots, t_n]$. Also $V'(t_j) = 0$, $j = 1, \ldots, n$, so that $V'(t)$ has $2n$ distinct zeros in (a, b). We deduce from Rolle's theorem that $V^{(2n)}(\xi) = 0$ for some $\xi \in (a, b)$. Since $t^n H_n(t)$ is a polynomial of degree $2n - 1$, it follows from (3.11) that $V^{(2n)}(\xi) = f^{(2n)}(\xi) - (2n)! K(x) = 0$, from which we obtain (3.10).

Integrating (3.10) and using (3.8) yields

$$\int_a^b F(t)\,\mathrm{d}\phi(t) = \sum_{k=1}^{n} w_k F(t_k) + \sum_{k=1}^{n} w'_k F'(t_k) + e_n^*(F) \tag{3.12}$$

where

$$w_k=\int_a^b S_{n,k}(t)\mathrm{d}\phi(t),\qquad w_k'=\int_a^b T_{n,k}(t)\mathrm{d}\phi(t),\quad k=1,2,\ldots,n, \tag{3.13}$$

and

$$e_n^*(F)=\frac{1}{(2n)!}\int_a^b f^{(2n)}(\xi(t))(t-t_1)^2\cdots(t-t_n)^2t^{-n}\mathrm{d}\phi(t). \tag{3.14}$$

It follows from (3.14) that $e_n^*(F)=0$ if $F\in\mathcal{R}_{2n-1}$. In particular, $e_n^*(H_n)=0$. Hereafter we let $t_j=t_j^{(n)}$, $j=1,\ldots,n$, where the $t_j^{(n)}$ are the zeros of $R_n^*(t)$. Then by the mean value theorem

$$e_n^*(F)=\frac{f^{(2n)}(\eta)}{k_n^2(2n)!}\int_a^b\mu_n\left[R_n^*(t)\right]^2\mathrm{d}\phi(t)=\frac{\delta(n)f^{(2n)}(\eta)}{k_n^2(2n)!}$$

where $a<\eta<b$ and $\mu_n=1$ for n even and $\mu_n=t$ for n odd. Thus it remains to show that $w_k=w_k^{(n)}$ and $w_k'=0$, $k=1,\ldots,n$. By (3.2) and (3.13)

$$w_k'=\int_a^b R_n^*(t)U(t)\mathrm{d}\phi(t)=0,\quad k=1,2,\ldots,n,$$

since $U(t)\in\mathcal{R}_{n-1}$. Finally we show that $w_k=w_k^{(n)}$. Since $H_n(t)\in\mathcal{R}_{2n-1}$, Theorem 2.3 implies that

$$\int_a^b H_n(t)\mathrm{d}\phi(t)=\sum_{j=1}^n w_j^{(n)}H_n\left(t_j^{(n)}\right)=\sum_{j=1}^n w_j^{(n)}F\left(t_j^{(n)}\right).$$

Replacing F by H_n in (3.12) yields

$$\int_a^b H_n(t)\mathrm{d}\phi(t)=\sum_{j=1}^n w_jH_n\left(t_j^{(n)}\right)=\sum_{j=1}^n w_jF\left(t_j^{(n)}\right),$$

so that

$$\sum_{j=1}^n w_jF\left(t_j^{(n)}\right)=\sum_{j=1}^n w_j^{(n)}F\left(t_j^{(n)}\right).$$

Since this holds with F replaced by $\Lambda_{n,k}$ and since $\Lambda_{n,k}(t_j)=\delta_{k,j}$ it follows that $w_j=w_j^{(n)}$, $j=1,\ldots,n$. □.

The following result relates Theorem 3.1 directly to the positive T-fraction expansion of Theorem 2.1.

Theorem 3.2. *Let $\phi(t)\in\Phi(a,b)$ with $0\leqslant a<b<+\infty$. Let $f_n(z)$ denote the nth approximant and $G(z)$ denote the limiting value of the positive T-fraction in Theorem 2.1. Then, for $z\in\mathbb{R}$, $z\notin[-b,-a]$,*

$$|G(z)-f_n(z)|\leqslant\frac{\delta(n)|z|^{n+1}}{k_n^2(a+z)^{2n+1}},\quad \text{if } z>-a, \tag{3.15a}$$

and

$$|G(z)-f_n(z)|<\frac{\delta(n)|z|^{n+1}}{k_n^2|b+z|^{2n+1}},\quad \text{if } z<-b \tag{3.15b}$$

where k_n^2 and $\delta(n)$ are defined by (3.5) *and* (3.7), *respectively.*

Proof. Let z be fixed, $F(t)=z/(z+t)$, $f(t)=t^nF(t)$. Then it is readily shown that

$$f^{(2n)}(t)=(-1)^n(2n)!z^{n+1}(t+z)^{-2n-1}.$$

Thus (3.15) follows immediately from Theorem 3.1. □

4. Applications to special functions

We consider here some examples of positive T-fraction (two-point Padé) expansions of analytic functions and compare them with analogous one-point Padé expansions.

Example 4.1. *Exponential integrals $E_n(w)$ are defined by*

$$E_n(w) = \int_1^{\infty}(e^{-wt}/t^n)dt, \quad \mathrm{Re}\, w > 0, \ n = 1, 2, 3, \ldots \tag{4.1}$$

We shall restrict attention to $E_1(w)$ since, by the relation $E_{n+1}(w) = [e^{-w} - wE_n(w)]n^{-1}$, the other $E_n(w)$ may be expressed in terms of $E_1(w)$. Taking $n = 1$ and $t = \sigma/w$ in (4.1) yields

$$E_1(w) = \int_w^{\infty}(e^{-\sigma}/\sigma)d\sigma, \quad |\arg w| < \pi. \tag{4.2}$$

Now letting $\sigma = \tau + \zeta$ in (4.2) and then $\tau = 1/t$ and $\zeta = 1/z = w - 1$, we obtain

$$E_1(w) = e^{1-w}G(1/(w-1)) \tag{4.3a}$$

where

$$G(z) = z\int_0^1 (t^{-1}e^{-1/t}/(z+t))dt. \tag{4.3b}$$

Here $G(z)$ is a holomorphic function of $z \notin [-1, 0]$ and has the form of the integral in Theorem 2.1, with $d\phi(t) = t^{-1}e^{-1/t}dt$ and $[a, b] = [0, 1]$. Hence $G(z)$ can be represented by a positive T-fraction (1.4). However, we prefer to consider a slightly different form for our expansion of $E_1(w)$. Using the partial fraction

$$\frac{1}{t(z+t)} = \frac{1}{z}\left[\frac{1}{t} - \frac{1}{z+t}\right]$$

and the fact that $E_1(1) = \int_0^1 t^{-1}e^{-1/t}dt$, we arrive at the expression

$$E_1(w) = e^{1-w}[E_1(1) + (1-w)T(1/(w-1))] \tag{4.4a}$$

where

$$T(z) = z\int_0^1 (e^{-1/t}/(z+t))dt. \tag{4.4b}$$

Here again $T(z)$ is a holomorphic function of z for $z \notin [-1, 0]$ and $T(z)$ has the form of the integral in Theorem 2.1 with $d\phi(t) = e^{-1/t}dt$ and $[a, b] = [0,1]$. The asymptotic expansions of $T(z)$ at $z = 0$ and

Table 1
Coefficients F_n, G_n in the positive T-fraction expansion of $T(z) = z\int_0^1 e^{-1/t}(z+t)^{-1}dt$ and coefficients k_n^2 from (3.5)

n	F_n	G_n	k_n^2
1	0.21938 39343 95520	1.4773 77593 15888	4.99×10^{1}
2	0.19949 74350 19818	2.1845 42949 64163	1.20×10^{3}
3	0.53148 29289 58047	2.6827 16184 27413	3.56×10^{3}
4	0.90407 05038 02134	3.0614 88067 61871	9.04×10^{4}
5	1.29831 67121 02766	3.4462 32969 30537	1.83×10^{5}
6	1.70630 98642 27231	3.7638 44895 71063	4.94×10^{6}
7	2.12395 98133 90531	4.0539 20731 93817	7.85×10^{6}
8	2.54884 29065 75927	4.3225 32863 72960	2.25×10^{8}
9	2.97939 09565 66136	4.5738 10230 86096	3.02×10^{8}
10	3.41452 36515 42848	4.8107 10385 91449	

$z = \infty$, respectively, with respect to the sectors $R_\alpha = [z\colon |\arg z| < \alpha]$, $0 < \alpha < \pi$ are given by (1.3). The coefficients in the positive T-fraction expansion

$$T(z) = \frac{F_1 z}{1 + G_1 z} + \frac{F_2 z}{1 + G_2 z} + \frac{F_3 z}{1 + G_3 z} + \cdots \tag{4.5}$$

can be obtained numerically by applying the FG-relations (1.5) and (1.6) to the double sequence of moments $\{c_n\}_{-\infty}^{\infty}$. The latter can be computed in terms of $\mu_k = (-1)^k c_k$ by first setting $\mu_0 = e^{-1} - E_1(1)$, where $E_1(1) = 0.21938\ 39343\ 95520\ 273665$ and then using the relations

$$\mu_k = e^{-1} - (k+2)\mu_{k+1}, \quad k = 0, \pm 1, \pm 2, \ldots$$

A sample of values of the coefficients F_n, G_n is in Table 1. Let $T_n(z)$ denote the nth approximant of (4.5). We shall study the approximations of $E_1(w)$ given by

$$E_{1,n}(w) = e^{1-w}\left[E_1(1) + (1-w)T_n(1/(w-1))\right], \quad n = 1, 2, 3, \ldots$$

Since $T_n(z)$ is the (n, n) two-point Padé approximant of $T(z)$, it is likely to approximate $T(z)$ best in neighborhoods of the points $z = 0$ and $z = \infty$. Therefore $E_{1,n}(w)$ is expected to approximate $E_1(w)$ best in neighborhoods of $w = 1$ and $w = \infty$. An application of (3.1) gives the *a posteriori* truncation error bounds (for $w \in (-\infty, 1)$)

$$|E_1(w) - E_{1,n}(w)| \leqslant K(w)|E_{1,n}(w) - E_{1,n-1}(w)| \tag{4.6a}$$

where

$$K(w) = \begin{cases} 1, & \text{if } \operatorname{Re} w \geqslant 1, \\ \csc|\arg(1/(w-1))|, & \text{if } \operatorname{Re} w < 1,\ w \notin \mathbb{R}. \end{cases} \tag{4.6b}$$

Applying Theorem 3.2 and (3.5) yields the *a priori* truncation error bounds

$$|E_1(w) - E_{1,n}(w)| \leqslant (w-1)^{n+1}/k_n^2 e^{w-1}, \quad \text{for } 1 < w < \infty, \tag{4.7a}$$

and

$$|E_1(w) - E_{1,n}(w)| \leqslant e^{1-w}(1-w)^{n+1}/k_n^2 w^{2n+1}, \quad \text{for } 0 < w < 1 \tag{4.7b}$$

Table 2
Truncation error $E_1(w) - E_{1,9}(w)$ and truncation error bounds for $E_{1,9}(w)$

w	$\lvert E_1(w) - E_{1,9}(w)\rvert$	Truncation error bounds	
		a priori from (4.7)	a posteriori from (4.6)
0.1	4.9×10^{-4}	2.8×10^{10}	Not applicable
0.2	7.1×10^{-6}	1.5×10^{4}	
0.3	2.0×10^{-7}	1.6×10^{0}	
0.4	6.9×10^{-8}	1.3×10^{-3}	
0.5	2.3×10^{-10}	2.8×10^{-6}	
0.6	6.2×10^{-12}	8.5×10^{-9}	
0.7	1.0×10^{-13}	2.3×10^{-11}	
0.8	2.5×10^{-15}	2.9×10^{-14}	
0.9	1.9×10^{-18}	2.7×10^{-18}	
1.1	1.1×10^{-20}	3.0×10^{-19}	1.9×10^{-18}
1.2	1.2×10^{-17}	2.8×10^{-16}	4.4×10^{-16}
1.3	2.9×10^{-16}	1.5×10^{-14}	7.9×10^{-15}
1.4	2.3×10^{-15}	2.3×10^{-13}	5.1×10^{-14}
1.5	1.0×10^{-14}	2.0×10^{-12}	1.9×10^{-13}
2.0	3.4×10^{-13}	1.2×10^{-9}	4.2×10^{-12}

where values of k_n^2, $n = 1, 2, \ldots, 10$ are included in Table 1. Some values of truncation error bounds for $E_{1,9}(w)$ obtained from (4.6) and (4.7) are given in Table 2. Also given for comparison are the actual absolute errors $|E_1(w) - E_{1,9}(w)|$. A posteriori bounds obtained by (4.6) are not applicable for $0 < w < 1$, but are seen to be quite sharp for the values given in the range $w > 1$. The a priori bounds obtained from (4.7) are not very sharp near the singular point $w = 0$ but are excellent in the neighborhood of the point of interpolation $w = 1$.

The convergence behavior of the sequence $\{E_{1,n}(w)\}$ can be described by means of contour maps of the number of significant digits $\mathrm{SD}(E_{1,n}(w))$ in the approximation of $E_1(w)$ by $E_{1,n}(w)$. For convenience we approximate $\mathrm{SD}(E_{1,n}(w))$ by

$$\widetilde{\mathrm{SD}}(E_{1,n}(w)) = -\log_{10}|(E_1(w) - E_{1,n}(w))/E_1(w)|.$$

In Figs. 1, 2 and 3 we give maps of constant level contours of $\widetilde{\mathrm{SD}}(E_{1,n}(w))$ in the square region of the w-plane, $|\mathrm{Re}(w)| \leqslant |w|$, $|\mathrm{Im}(w)| \leqslant 20$, for each of the fixed values of $n = 5$, 7 and 10. These maps were produced using the NCAR plotting package of the National Center for Atmospheric Research. (A slight amount of smoothing was introduced by a draftsman.) An expected characteristic suggested by these maps is that the approximations of $E_1(w)$ are best near $w = 1$ and $w = \infty$. The maps indicate that, for sufficiently large $|w|$, $\mathrm{SD}(E_{1,n}(w))$ increases monotonically with $|w|$ along fixed rays $|\arg w| =$ constant. The symmetry with respect to the real axis is due to the fact that $E_1(w)$ and $E_{1,n}(w)$ are defined by real coefficients. This symmetry is of interest since the function $E_1(w)$ has a discontinuity (like $\log w$) as w approaches the negative real axis from above and from below. The speed of convergence of $E_{1,n}(w)$ can be ascertained approximately by comparing the maps for different values of n.

We wish now to compare the approximation $E_{1,n}(w)$ with an expansion of $E_1(w)$ by ordinary (one-point) Padé approximants. Letting $\sigma = w + t$ in (4.2) yields

$$E_1(w) = \frac{e^{-w}}{w} H(w) \quad \text{where} \quad H(w) = w \int_0^\infty \frac{e^{-t}}{w+t} \mathrm{d}t. \tag{4.8}$$

Here $H(w)$ has the form of the integral (1.2), where $\mathrm{d}\phi(t) = e^{-t}\mathrm{d}t$, $[a, b) = [0, \infty]$ and hence $\phi(t) \in \Phi^c(0,$

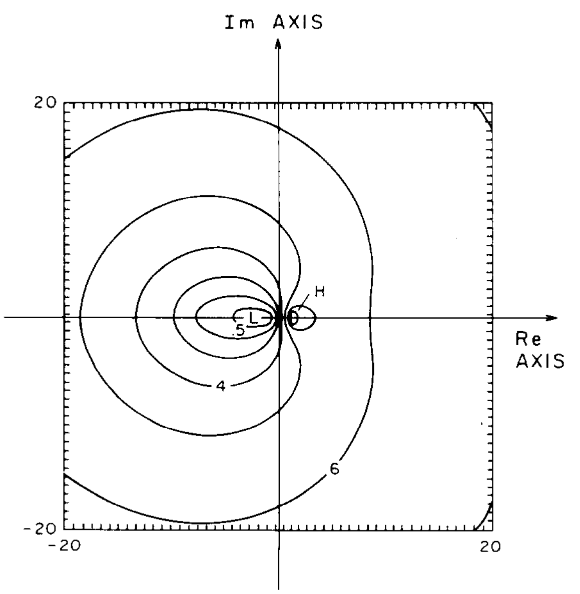

Fig. 1. Contours of constant levels of the number of significant digits $\widetilde{\mathrm{SD}}(E_{1,5}(w))$ in the approximation of the exponential integral $E_1(w)$ by the two-point Padé approximant $E_{1,5}(w)$.

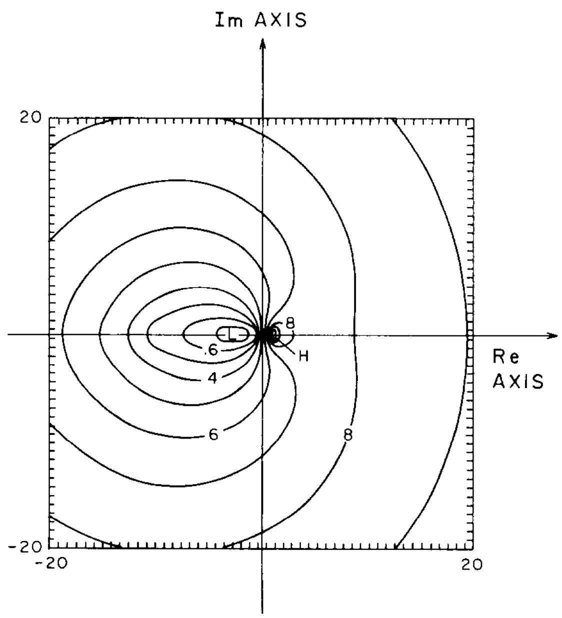

Fig. 2. Contours of constant levels of the number of significant digits $\widetilde{\mathrm{SD}}$ $(E_{1,7}(w))$ in the approximation of the exponential integral $E_1(w)$ by the two-point Padé approximant $E_{1,7}(w)$.

∞). It follows that $H(w)$ has the asymptotic expansion

$$L_\infty^* = \sum_{n=0}^{\infty} (-1)^n n! w^{-n} \tag{4.9}$$

at $w = \infty$ with respect to $R_\alpha = [w\colon |\arg w| < \alpha]$, $0 < \alpha < \pi$. Applying the qd-algorithm to L_∞^* yields

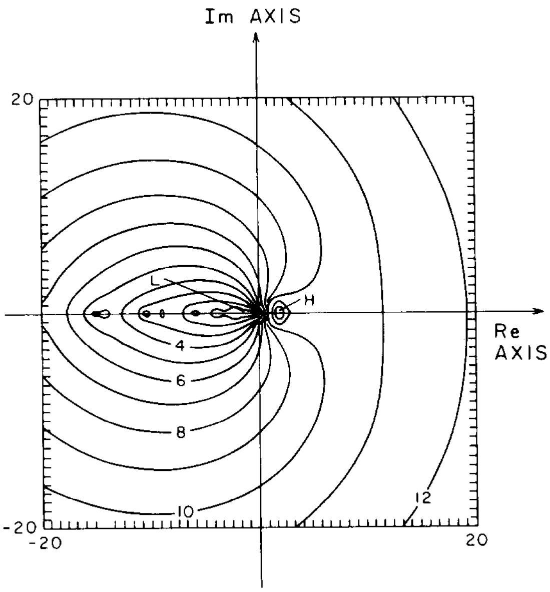

Fig. 3. Contours of constant levels of the number of significant digits $\widetilde{\mathrm{SD}}(E_{1,10}(w))$ in the approximation of the exponential integral $E_1(w)$ by the two-point Padé approximant $E_{1,10}(w)$.

$e_m^{(n)} = -1$ for $n \geqslant 0$, $m \geqslant 1$ and $q_m^{(n)} = -(n+m)$ for $n \geqslant 0$, $m \geqslant 0$. Thus we arrive at the modified S-fraction

$$\frac{1}{1} + \frac{1}{w} + \frac{1}{1} + \frac{2}{w} + \frac{1}{1} + \frac{3}{w} + \cdots \tag{4.10}$$

corresponding to L_∞^* at $w = \infty$. By the convergence criterion (1.4) this continued fraction is convergent and we obtain

$$E_1(w) = \frac{e^{-w}}{w}\left[\frac{1}{1} + \frac{1}{w} + \frac{1}{1} + \frac{2}{w} + \frac{1}{1} + \frac{3}{w} + \cdots\right], \quad |\arg w| < \pi, \tag{4.11}$$

or by an equivalence transformation

$$E_1(w) = e^{-w}\left[\frac{1}{w} + \frac{1}{1} + \frac{1}{w} + \frac{2}{1} + \frac{1}{w} + \frac{3}{1} + \cdots\right], \quad |\arg w| < \pi. \tag{4.12}$$

Now let $h_n(w)$ denote the nth approximant of the continued fraction (in brackets) in (4.12) and let $H_n(w) = e^{-w} h_n(w)$. We recall that $h_{2m}(w)$ is the $(m-1,\ m)$ (and $h_{2m+1}(w)$ is the $(m,\ m)$) Padé approximant of $e^w E_1(w)$. In order to compare the approximations $E_{1,10}(w)$ and $H_{20}(w)$, we give in Fig. 4 the graphs of $\widetilde{\mathrm{SD}}(E_{1,10}(w))$ and $\widetilde{\mathrm{SD}}(H_{20}(w))$ for real values of w in the range $0 < w \leqslant 100$. As expected, $E_{1,10}(w)$ is better than $H_{20}(w)$ for $0.1 \leqslant w \leqslant 6$, whereas the reverse is true for $7 \leqslant w \leqslant 100$. Nevertheless $E_{1,10}(w)$ gives at least 10 significant digits for $w \geqslant 0.5$, so that for practical purposes the two-point Padé approximant seems to be better than the one-point Padé approximant. The computations for this illustration were performed on a CDC Cyber with double-precision arithmetic (i.e. about 28 decimal digits).

We note that, whereas the coefficients in the continued fraction of (4.8) can be expressed by a simple function of n, no such simple expression is known for the coefficients F_n and G_n (Table 1). However, the F_n

and G_n can be generated numerically by a rather simple program involving the recurrence relations for the moments c_k and the FG-algorithm (1.5) and (1.6). A similar situation holds for the Stieltjes fraction expansion for $\log \Gamma(z)$ [19, pp. 348–350], which, nevertheless, is considered to give useful approximations.

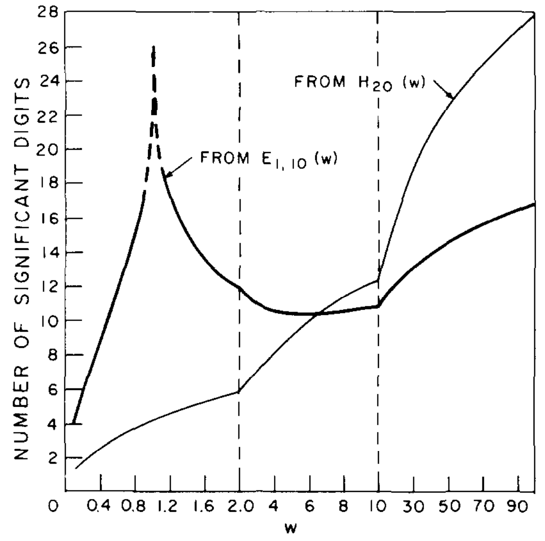

Fig. 4. Number of significant digits obtained in approximations of the exponential integral $E_1(w)$ by the two-point Padé approximant $E_{1,10}(w)$ and the one-point Padé approximant $H_{20}(w)$.

Example 4.2. The *natural logarithm*

$$\log w = \int_1^w \mathrm{d}t/t \tag{4.13}$$

can be written in the form

$$\log w = z^{-1}G(z) = \left(\frac{1}{w-1} - \delta\right)^{-1} G\left(\frac{1}{w-1} - \delta\right) \tag{4.14}$$

where

$$G(z) = z\int_\delta^{1+\delta} \frac{\mathrm{d}t}{z+t}, \quad z = \frac{1}{w-1} - \delta, \quad \delta > 0, \tag{4.15}$$

after making the succession of transformations in (4.13): $t = \tau + 1$, $\tau = (w-1)u$, $u = t + \delta$. Since (4.15) has the form of the integrals considered in Theorem 2.1., the function $G(z)$ has a positive T-fraction representation

$$G(z) = \frac{F_1 z}{1 + G_1 z} + \frac{F_2 z}{1 + G_2 z} + \frac{F_3 z}{1 + G_3 z} + \cdots \tag{4.16}$$

valid for all $z \notin [-(1+\delta), -\delta]$ (that is, for all $w \in \mathbb{C} - (-\infty, 0]$). In the following, the discussion is restricted to the special case in which $\delta = (\mathrm{e}-1)^{-1}$. We then have

$$G(z) = z\int_a^b \frac{\mathrm{d}t}{z+t}, \quad z = \frac{1}{w-1} - \frac{1}{\mathrm{e}-1} \tag{4.17}$$

where $a = (\mathrm{e}-1)^{-1}$ and $b = \mathrm{e}/(\mathrm{e}-1)$. If $g_n(z)$ denotes the nth approximant of (4.16), then

$$F_n(w) = \left(\frac{1}{w-1} - \frac{1}{\mathrm{e}-1}\right)^{-1} g_n\left(\frac{1}{w-1} - \frac{1}{\mathrm{e}-1}\right)$$

Table 3
Coefficients in the positive T-fraction (two-point Padé approximant) expansion of $G(z)=z\int_a^b(z+t)^{-1}\mathrm{d}t$, $a=(\mathrm{e}-1)^{-1}$, $b=\mathrm{e}/(\mathrm{e}-1)$

n	F_n	G_n
1	1.000000 00000	0.10000 00000
2	0.086161 26963	0.10510 45753
3	0.071404 24451	0.10433 20240
4	0.068467 96285	0.10425 83248
5	0.067582 94758	0.10423 69916
6	0.067187 29482	0.10422 87384
7	0.066975 97268	0.10422 48745
8	0.066849 74480	0.10422 28254
9	0.066768 31795	0.10422 16378
10	0.066712 72181	0.10422 09021

Table 4
Number of significant digits $\mathrm{SD}(F_n(w))$ in approximation in $\log w$ by $F_n(w)$. The calculations were performed by a CDC Cyber in double precision (approximately 28 decimal digit) arithmetic

w	$\mathrm{SD}(F_5(w))$	$\mathrm{SD}(F_{10}(w))$
1.0	11.2	22.6
1.3	9.4	19.0
1.5	9.0	18.1
1.7	8.9	17.9
1.9	9.1	18.3
2.1	9.5	19.1
2.3	10.2	20.5
2.5	11.5	23.1
2.7	16.8	24.8

is the resulting nth approximant of $\log w$. The moments $c_k=(-1)^k\mu_k$ corresponding to (4.17) are given by

$$\mu_k=\begin{cases}1, & \text{if } k=-1,\\ \dfrac{\mathrm{e}^{n+1}-1}{(n+1)(\mathrm{e}-1)^{n+1}}, & \text{if } k\neq -1.\end{cases}$$

Using these and the FG-relations (1.5) and (1.6), once can compute the coefficients F_n, G_n in (4.16). A sample of the coefficients is given in Table 3. From this it appears that the continued fraction (1.4) may be limit periodic (i.e. the sequences $\{F_n\}$ and $\{G_n\}$ may converge). Since the two-point Padé approximant $g_n(t)$ interpolates to L_0 and L_∞ (see (1.3)) at $z=0$ and $z=\infty$, respectively, the approximation $F_n(w)$ is expected to be best near $w=\mathrm{e}$ and $w=1$. This justifies the choice of $\delta=(\mathrm{e}-1)^{-1}$ above, since $[1, \mathrm{e}]$ is a fundamental interval for $\log w$ (in the sense that all values of the function can be obtained if we know $\log w$ for $1\leqslant w\leqslant \mathrm{e}$). The convergence behavior is illustrated by the values of $\widetilde{\mathrm{SD}}(F_n(w))$ for $1\leqslant w\leqslant \mathrm{e}$ given in Table 4.

Examples 4.3. The *inverse tangent*

$$\operatorname{Arctan} w=\int_0^w \mathrm{d}u/(1+u^2) \tag{4.18}$$

can be written in the form

$$\operatorname{Arctan} w=\frac{w}{2(1-w^2)}G\left(\frac{1}{w^2}-1\right) \tag{4.19}$$

where

$$G(z)=z\int_1^2\frac{(t-1)^{-1/2}\mathrm{d}t}{z+t},\quad z=\frac{1}{w^2}-1 \tag{4.20}$$

after making the succession of transformations in (4.18): $u=wv$, $v=\tau^{1/2}$, $\tau=t-1$. Since (4.20) has the form of the integrals considered in Theorem 2.1, the function $G(z)$ has a positive T-fraction representation (2.1) valid for $z\notin[-2, -1[$ (that is, for $w\notin[-\mathrm{i}, \mathrm{i}\infty)$ and $w\notin[-\mathrm{i}, -\mathrm{i}\infty)$). Since $w=1$ when $z=0$ and $w=0$ when $z=\infty$, the resulting approximants of $\operatorname{Arctan} w$ will be best near $w=0$ and $w=1$. No numerical results are given for this example, but the procedures are the same as in Examples 4.1. and 4.2.

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