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Padé Approximation of Stieltjes Series

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Using Nuttall's compact formula for the $[n, n-1]$ Padé approximant, the authors show that there is a natural connection between the Padé approximants of a series of Stieltjes and orthogonal polynomials. In particular, we obtain the precise error formulas. The $[n, n-1]$ Padé approximant in this case is just a Gaussian quadrature of the Stieltjes integral. Hence, analysis of the error is now possible and under very mild conditions it is shown that the $[n, n+j]$, $j \geq -1$, Padé approximants converge to the Stieltjes integral.

1. INTRODUCTION

This paper is concerned with properties of the diagonal Padé approximants of Stieltjes series. In particular we develop a natural connection between the diagonal Padé approximants and systems of orthogonal polynomials using the compact formula of Nuttall (which we have generalized in [1]). Secondly, we give some error formulae in terms of these polynomials. Finally, observing the connection between the Padé approximants and Gaussian quadrature for the measure in the Stieltjes integral

$$\int_0^\infty \frac{d\sigma(t)}{1 - tz} \tag{1.1}$$

whose formal power series is our Stieltjes series, we prove that the diagonal Padé approximants converge uniformly to the integral (1.1) on compact sets disjoint from the interval $[0, \infty)$. The proof is relatively elementary and, unlike Baker's, does not use determinant theory. (Baker [3] proves only that the Padé approximants converge).

The connection between orthogonal polynomials and Padé approximants has been observed by Wheeler and Gordon [4, p. 99–128] who have investigated approximants of the integral

$$\int_0^\infty F(t)\, d\sigma(t),$$

where σ is a bounded positive measure and $F(t) \in C[0, \infty)$. This problem includes (1.1) because $F(t)$ is permitted to have parametric dependence on any number of variables. In a more recent paper, Bessis [5] makes similar observations in a holomorphic operator setting.

We derive our results using independent and elementary proofs, and in particular we prove convergence. Also, we give an application of the Padé approximant method to an irregular singular point problem in the theory of differential equations.

We start with a brief description of Padé approximation. The idea is simple: Given a formal power series

$$f(z) = a_0 + a_1 z + a_2 z^2 + \cdots,$$

$a_0 \neq 0$, let $Q(z) = q_0 + q_1 z + \cdots + q_n z^n$ and $P(z) = p_0 + p_1 z + \cdots + p_m z^m$ be polynomials of degrees no greater than n and m, respectively. We wish to determine the constants $q_0, \ldots, q_n$ and $p_0, \ldots, p_m$ so that (1.2) holds for the formal power series on its left:

$$f(z)\,Q(z) - P(z) = d_{m+n+1} z^{m+n+1} + \cdots. \tag{1.2}$$

This requires that the constants p_i and q_i satisfy

$$\sum_j a_{l-j} q_j - p_l = 0, \qquad l = 0, \ldots, m,$$

$$\sum_j a_{l-j} q_j = 0 \qquad l = m+1, \ldots, m+n.$$

A rank argument shows that this system can always be solved nontrivially. In fact, the ratio $P(z)/Q(z)$ is given by Baker [3], namely,

$$\frac{P(z)}{Q(z)} = [n, m](z) = \frac{\begin{vmatrix} a_{m-n+1} & a_{m-n+2} & \cdots & a_{m+1} \\ \vdots & \vdots & & \\ a_m & a_{m+1} & & \\ \sum\limits_{j=n}^{m} a_{j-n} z^j & \sum\limits_{j=n-1}^{m} a_{j-n+1} a^j & \cdots & \sum\limits_{j=0}^{m} a_j z^j \end{vmatrix}}{\begin{vmatrix} a_{m-n+1} & a_{m-n+2} & \cdots & a_{m+1} \\ \vdots & & & \\ a_m & a_{m+1} & & a_{m+n} \\ z^n & z^{n-1} & \cdots & 1 \end{vmatrix}},$$

when the determinant in the denominator is nonzero. Here, $[n, m](z)$ denotes the $[n, m]$ Padé approximant to $f(z)$.

It was observed recently by Gragg [10] that the form (1.2) is equivalent to the form

$$f(z) - \frac{P(z)}{Q(z)} = O(z^{\nu}) \qquad \text{as} \quad z \to 0, \tag{1.3}$$

where $P(z)$ and $Q(z)$ are polynomials of degrees less than or equal to m and n, respectively, and ν is as large as possible.

In the case of series of Stieltjes, the formal power series for the integral (1.1) is $\sum_{j=0}^{\infty} a_j z^j$ where the coefficients a_j are the moments of the positive measure $d\sigma(t)$,

$$a_j = \int_0^{\infty} t^j \, d\sigma(t).$$

To eliminate trivial cases, the corresponding function $\sigma(t)$ is assumed to have infinitely many points of increase. It is well known [2] that the sequence $\{a_n\}$ and $\sigma(t)$ uniquely determine one another.

2. Orthogonal Polynomials and Padé Approximants

Let ϕ be an increasing real-valued function on $[0, \infty)$, with infinitely many points of increase. Then the measure $d\phi$ is positive on $[0, \infty)$. If we assume that all the moments

$$a_j = \int_0^{\infty} t^j \, d\phi \tag{2.1}$$

are finite, the formal power series

$$\sum_{j=0}^{\infty} a_j z^j \tag{2.2}$$

is called a series of Stieltjes. In a natural way this formal power series is associated with the function

$$f(z) = \int_0^{\infty} \frac{d\phi(t)}{1 - zt}. \tag{2.3}$$

Note that in many papers on Padé approximation (e.g., Baker [3]) the integral in (2.3) is defined with $-z$ instead of z. We feel, however, that the resulting formulas are simpler with the form of the integral used in (2.3). Let $\{L_k\}$, $k = 0, 1, \ldots$, be the orthonormal set of polynomials with respect to the measure $d\phi$ with positive leading coefficients. That is, L_k is a polynomial of exact degree k, say

$$L_k(t) = \sum_{j=0}^{k} l_j^k t^j, \qquad l_k^k > 0, \qquad \text{for} \quad k = 1, 2, \ldots, \tag{2.4}$$

and

$$\int_0^\infty L_k L_j \, d\phi = \delta_{kj}\,, \tag{2.5}$$

where δ_{kj} is the usual Kronecker delta.

We can now state two theorems which demonstrate the intimate connection between orthogonal polynomials and Padé approximants.

THEOREM 2.1. *The* $[n, n-1]$ *Padé approximant to the Stieltjes series* $\sum_{j=0}^{\infty} a_j z^j$ *is given by*

$$[n, n-1](z) = P(z)/Q(z), \tag{2.6}$$

where

$$Q(z) = z^n L_n(z^{-1}) = \sum_{k=0}^{n} l_{n-k}^n z^k,$$

$$P(z) = \sum_{k=0}^{n-1} z^k \sum_{j=n-k}^{n} l_{2n-j-k}^n a_{n-j}\,, \tag{2.7}$$

and the $l_k{}^n$ *are the coefficients of the orthogonal polynomial* L_n *of degree* n *given in* (2.4).

We postpone a proof of this theorem, but we note an immediate and interesting corollary which was proved by Baker [3].

COROLLARY 2.1. *The poles of the* $[n, n-1]$ *Padé approximant to* (2.2) *are simple and lie on the positive real axis. Furthermore, if* $x_1, \ldots, x_n$ *are the poles of the* $[n, n-1]$ *Padé approximant and* $y_1, \ldots, y_{n+1}$ *are the poles of the* $[n+1, n]$ *Padé approximant then*

$$y_1 < x_1 < y_2 < \cdots < x_n < y_{n+1}\,. \tag{2.8}$$

To prove this corollary, we factor z^n out of the denominator of (2.6) to obtain $z^n(L_n(z^{-1}))$. Thus the denominator vanishes at the reciprocals of the n zeroes of the orthogonal polynomial L_n. It is well known [7] that L_n has n simple zeroes in $(0, \infty)$. It is also known [7] that the zeroes of L_n interlace the zeroes of L_{n+1} in the sense of (2.8). This clearly implies that the zeroes of $z^n L_n(z^{-1})$ and $z^{n+1} L_{n+1}(z^{-1})$ interlace as well.

The second theorem which we wish to state gives an exact formula for the error term in the $[n, n-1]$ Padé approximant and, as an immediate consequence, an important formula for $[n, n-1](z)$.

THEOREM 2.2. *The error in approximating $f(z)$ with $[n, n-1](z)$ is given by*

$$f(z) - [n, n-1](z) = \frac{1}{L_n(z^{-1})} \int_0^\infty \frac{L_n(t)}{1 - zt} \, d\phi(t) \tag{2.9}$$

or by

$$f(z) - [n, n-1](z) = \frac{z^{2n}}{z^n L_n(z^{-1})} \int_0^\infty \frac{t^n L_n(t)}{1 - zt} \, d\phi(t). \tag{2.10}$$

In addition, the $[n, n-1]$ Padé approximant is given by

$$[n, n-1](z) = \frac{1}{L_n(z^{-1})} \int_0^\infty \frac{L_n(z^{-1}) - L_n(t)}{1 - zt} \, d\phi(t). \tag{2.11}$$

We will now prove Theorems 2.1 and 2.2.

Proof of Theorem 2.1. The equation for the $[n, n-1]$ Padé approximant to the Stieltjes series (2.2), obtained by Nuttall [4, p. 219], is given by

$$[n, n-1](z) = \hat{c}_n{}^T \hat{a}_n, \tag{2.12}$$

where $\hat{a}_n = (a_0, a_1, ..., a_{n-1})^T$ and $\hat{c}_n = (c_0, c_1, ..., c_{n-1})^T$ satisfy

$$M_n(z)\, \hat{c}_n = \hat{a}_n \tag{2.13}$$

and

$$M_n(z) = \begin{pmatrix} a_0 - za_1 & \cdots & a_{n-1} - za_n \\ \vdots & & \vdots \\ a_{n-1} - za_n & \cdots & a_{2n-2} - za_{2n-1} \end{pmatrix}. \tag{2.14}$$

We first note that $M_n(z)$ has the simple form

$$M_n(z) = \int_0^\infty (1 - zt)\, \hat{\tau}(t)\, \hat{\tau}(t)^T \, d\phi(t), \tag{2.15}$$

where $\hat{\tau}(t) = (1, t, t^2, ..., t^{n-1})^T$. Also,

$$\hat{a}_n = \int_0^\infty \hat{\tau}(t)\, d\phi(t). \tag{2.16}$$

Thus, we see that Eq. (2.13) is equivalent to

$$\begin{aligned} 0 &= \int_0^\infty [(1 - zt)\, \hat{\tau}(t)\, \hat{\tau}(t)^T \hat{c}_n - \hat{\tau}(t)]\, d\phi(t) \\ &= \int_0^\infty \hat{\tau}(t)[(1 - zt)\, \hat{\tau}(t)^T \hat{c}_n - 1]\, d\phi(t) \\ &= \int_0^\infty \hat{\tau}(t)\, P_n(t)\, d\phi(t). \end{aligned} \tag{2.17}$$

We see immediately from (2.17) that $P_n(t)$ is orthogonal to the set $\{1, t, t^2,..., t^{n-1}\}$. Since $P_n(t)$ is a polynomial of degree n or less, it follows that $P_n(t)$ must be a constant multiple of L_n. That is,

$$P_n(t) = \beta L_n(t) = \beta \sum_{j=0}^{n} l_j^n t^j. \tag{2.18}$$

Equating like powers, we obtain $\beta = -c_{n-1}z/l_n^n$ and

$$\begin{gathered} c_0 + z(l_0^n/l_n^n)\, c_{n-1} = 1 \\ -zc_{j-1} + c_j + z(l_j^n/l_n^n)\, c_{n-1} = 0, \qquad j = 1,..., n-1. \end{gathered} \tag{2.19}$$

Solving for the c_j's yields, for $j = 1,..., n$,

$$c_{n-j} = \left(\sum_{k=n-j}^{n-1} l_{2n-j-k}^n z^k\right) \Big/ \left(\sum_{k=0}^{n} l_{n-k}^n z^k\right). \tag{2.20}$$

The Padé approximant is then given by

$$\begin{aligned} [n, n-1](z) &= \sum_{j=1}^{n} c_{n-j} a_{n-j} \\ &= P(z)/Q(z), \end{aligned} \tag{2.21}$$

where $P(z)$ and $Q(z)$ are obviously given by formulae (2.7). Q.E.D.

Proof of Theorem 2.2. Consider the difference

$$\begin{aligned} &f(z) - [n, n-1](z) \\ &= \frac{1}{z^n L_n(z^{-1})} \int_0^\infty \left[\frac{z^n L_n(z^{-1}) - (1 - zt)(\sum_{k=0}^{n-1} z^k \sum_{j=n-k}^{n} l_{2n-j-k}^n t^{n-j})}{1 - zt}\right] d\phi(t), \end{aligned} \tag{2.22}$$

which follows from (2.7), (2.1), and (2.3). Let $F(z, t)$ be the numerator of the integrand in (2.22). Clearly, $F(z, t)$ may be written as

$$\begin{aligned} F(z, t) &= \sum_{k=0}^{n} l_{n-k} z^k - \sum_{k=0}^{n-1} z^k \sum_{j=n-k}^{n} l_{2n-j-k}^n t^{n-j} + \sum_{k=0}^{n-1} z^{k+1} \sum_{j=n-k}^{n} l_{2n-j-k}^n t^{n-j+1} \\ &= I_1 + I_2 + I_3. \end{aligned}$$

In the third term above, I_3, let $k' = k + 1, j' = j - 1$, then I_3 has the form

$$\begin{aligned} I_3 &= \sum_{k'=1}^{n} z^{k'} \sum_{j'=n-k'}^{n-1} l_{2n-j'-k'}^n t^{n-j'} \\ &= \sum_{k'=1}^{n-1} z^{k'} \sum_{j'=n-k'}^{n-1} l_{2n-j'-k'}^n t^{n-j'} + z^n \sum_{j'=0}^{n-1} l_{n-j'}^n t^{n-j'}. \end{aligned}$$

Also, the second term I_2 has the form

$$I_2 = \sum_{k=0}^{n-1} z^k \sum_{j=n-k}^{n-1} l_{2n-j-k}^n t^{n-j} + \sum_{k=0}^{n-1} z^k l_{n-k}^n .$$

Combining all these three terms I_1, I_2, and I_3, we have that

$$\begin{aligned} F(z, t) &= z^n l_0{}^n + z^n \sum_{j=0}^{n-1} l_{n-j}^n t^{n-j} \\ &= z^n L_n(t). \end{aligned} \tag{2.23}$$

Hence, (2.9) follows immediately from (2.22) and (2.23).

To establish (2.10), we note that

$$\frac{1}{1 - zt} = \sum_{j=0}^{n-1} t^j z^j + \frac{z^n t^n}{1 - zt} .$$

By (2.9),

$$\begin{aligned} f(z) - [n, n-1](z) &= \frac{1}{L_n(z^{-1})} \sum_{j=0}^{n-1} z^j \int_0^\infty t^j L_n(t)\, d\phi(t) \\ &\quad + \frac{z^{2n}}{z^n L_n(z^{-1})} \int_0^\infty \frac{t^n L_n(t)\, d\phi(t)}{1 - zt} . \end{aligned}$$

Since $L_n(t)$ is orthogonal to all polynomials of degree less than n,

$$\int_0^\infty t^j L_n(t)\, dt = 0, \qquad j = 0, \ldots, n-1.$$

Using this fact in the previous formula, we obtain (2.10).

Finally, we remark that (2.11) follows immediately from (2.9) and (2.3). Q.E.D.

3. Gaussian Quadrature Formulas

We have just seen the remarkable connection between the $[n, n-1]$ Padé approximants and orthogonal polynomials. It is also interesting and uesful then to learn that the $[n, n-1]$ Padé approximant of the Stieltjes series (2.2) is exactly the nth order Gaussian quadrature approximation to the integral (2.3).

THEOREM 3.1. *The* $[n, n-1]$ *Padé approximant of* (2.2) *is the Gaussian quadrature approximation to* (2.3). *That is,*

$$[n, n-1](z) = \sum_{k=1}^{n} \frac{\alpha_{nk}}{1 - zx_k} \doteq \int_0^\infty \frac{d\phi}{1 - zt}, \tag{3.1}$$

where the $x_k = x_k^{(n)}$, $k = 1,..., n$ *are the zeroes of* L_n *and the* α_{nk} *are the Gaussian weights* (*Cotes numbers or Christoffel numbers*).

For more information on Gaussian quadrature the reader may consult Davis [5], Davis and Rabinowitz [7], and Stroud and Secrest [11]. One of the very important facts about Gaussian quadrature is that the weights, α_{nk}, are positive and sum to $\int_0^\infty d\phi$. This fact alone yields an easy proof of the following result due to Baker [3].

COROLLARY 3.1. *The set* $\{[n, n-1](z)\}$, $n = 1, 2,...,$ *is a normal family in the cut complex plane* $C\backslash[0, \infty)$ *and the residues of* $[n, n-1](z)$ *are all negative.*

We first use Corollary 3.1 to prove Corollary 3.2 below. Since the function $g(t) = 1/(1 - zt)$ is bounded and continuous on $[0, \infty)$ for each $z \notin [0, \infty)$, it follows by arguments similar to those in Uspensky [12] that under rather mild conditions the Gaussian quadrature approximation to $\int_0^\infty g(t)\, d\phi$ converges for each fixed z. This observation combined with Corollary 3.1 will yield a proof of Corollary 3.2.

COROLLARY 3.2. *The sequence* $\{[n, n-1](z)\}$ *converges uniformly on compact subsets of the cut complex plane* $C\backslash[0, \infty)$ *to*

$$f(z) = \int_0^\infty \frac{d\phi}{1 - zt}$$

if the moments a_m *satisfy* $a_m = O((2m + 1)!\, R^{2m})$ *for some* $R > 0$.

Proof of Theorem 3.1. We first calculate the residues of $[n, n-1](z)$. Let x_j^* be a pole of the Padé approximant. By Corollary 2.1, $x_j = 1/x_j^*$ is a zero of $L_n(t)$ so that

$$\begin{aligned}
\lim_{z \to x_j^*} (z - x_j^*)[n, n-1](z) &= \lim_{z \to x_j^*} \frac{(z - x_j^*)}{L_n(z^{-1})} \int_0^\infty \frac{L_n(z^{-1}) - L_n(t)}{1 - zt}\, d\phi \\
&= \lim_{w \to x_j} \frac{((1/w) - (1/x_j))}{L_n(w)} \int_0^\infty \frac{L_n(w) - L_n(t)}{1 - t/w}\, d\phi \\
&= \frac{1}{L_n'(x_j)}\, x_j^* \int_0^\infty \frac{L_n(t)}{x_j - t}\, d\phi \\
&= -x_j^* \alpha_{nj}, \qquad (3.2)
\end{aligned}$$

where α_{nj} is the weight corresponding to x_j in the Gaussian formula (see for example Davis [6, p. 343]). This result follows since

$$L_n(t)/[(t - x_j) L'(x_j)] \tag{3.3}$$

is the Lagrange polynomial of degree $n - 1$ interpolating 0 at $\{x_i\}_{i \neq j}$ and 1 at x_j. Thus

$$\begin{aligned} [n, n-1](z) &= \sum_{j=1}^{n} \frac{-\alpha_{nj} x_j^*}{z - x_j^*} \\ &= \sum_{j=1}^{n} \frac{\alpha_{nj}}{1 - z x_j}, \end{aligned} \tag{3.4}$$

which is the Gaussian approximation to the integral (2.3). Q.E.D.

We have just shown in calculation (3.2) that the residues of the Padé approximants are negative. This observation proves the second portion of Corollary 3.1. We now complete the proof of Corollary 3.1. Using the partial fractions decomposition obtained in (3.4) we see that

$$|1 - z x_j| \geqslant \begin{cases} 1 - x_j \operatorname{Re}(z) \geqslant 1 & \text{if} \quad \operatorname{Re}(z) \leqslant 0 \\ |\operatorname{Im}(z)|/|z|, & z \neq 0. \end{cases} \tag{3.5}$$

The second inequality follows by observing that x_j is real and $|1 - z x_j| = |z|\,|(1/z) - x_j|$. Hence

$$|[n, n-1](z)| \leqslant \sum_{j=1}^{n} \frac{\alpha_j}{|1 - z x_j|} \leqslant \begin{cases} \sum_{i=1}^{n} \alpha_j = \int_0^\infty d\phi, & \operatorname{Re}(z) \leqslant 0 \\ (|z|/|\operatorname{Im}(z)| \int_0^\infty d\phi, & \operatorname{Im} z \neq 0. \end{cases} \tag{3.6}$$

Therefore, $[n, n-1](z)$ is uniformly bounded on compact subsets of $\mathbb{C}\backslash[0, \infty]$ and is thus a normal family by Montel's theorem, proving Corollary (3.1). Q.E.D.

Corollary 3.2 now follows easily by Vitali's theorem and the fact that the quadrature approximations converge pointwise to

$$f(z) = \int_0^\infty \frac{d\phi}{1 - zt}.$$

This is slightly stronger than Baker's result since we know what the Padé approximants converge to. This completes the discussion of the $[n, n-1]$ Padé. We now turn to the $[n, n+j]$ Padé approximant.

4. The $[n, n+j]$ Padé Approximants

The results of the previous sections may be extended quite naturally to cover the $[n, n+j]$ Padé approximants where $j \geqslant -1$. In fact, we will see that the $[n, n+j]$ Padé approximant of the Stieltjes series (2.2) is just a fixed polynomial of degree j plus z^{j+1} times an $[n, n-1]$ Padé approximant of another Stieltjes series [1]. That is, let

$$f_j(z) = \int_0^\infty \frac{t^{j+1}\, d\phi}{1 - zt} = \int_0^\infty \frac{1}{1 - zt}\, d\phi_j\,. \tag{4.1}$$

Then $f_j(z)$ is associated with the Stieltjes series

$$\sum_{k=0}^{\infty} a_k^{(j)} z^k = \sum_{k=0}^{\infty} a_{k+j} z^j, \tag{4.2}$$

where $a_k^{j)} = \int_0^\infty t^k\, d\phi_j = \int_0^\infty t^{k+j}\, d\phi$. Denoting by $[n, m]_j(z)$ the $[n, m]$ Padé approximant of the series (4.2) we see that

$$[n, n+j](z) = \sum_{l=0}^{j} a_l z^l + z^{j+1}[n, n-1]_j\,(z). \tag{4.3}$$

We can therefore transfer all the results collected in Sections 2 and 3 to the $[n, n+j]$ case where $j \geqslant -1$. Thus we obtain the following results:

Theorem 4.1. *The $[n, n+j]$ Padé approximant to the Stieltjes series $\sum_{j=0}^{\infty} a_j z^j$ is given by*

$$[n, n+j](z) = \sum_{l=0}^{j} a_l z^l + P(z)/Q(z) \tag{4.4}$$

where

$$\begin{aligned} Q(z) &= z^n L_n(z^{-1}) = \sum_{k=0}^{n} l_{n-k}^n z^k, \\ P(z) &= \sum_{k=0}^{n-1} z^k \sum_{j=n-k}^{n} l_{2n-j-k}^n a_{n-j}\,, \end{aligned} \tag{4.5}$$

and where L_n is the orthogonal polynomial of degree n with respect to the measure $d\phi_j$ and $L_n(z) = \sum_{k=0}^{n} l_k{}^n z^k$.

Corollary 2.1 becomes in this general case:

Corollary 4.1. *The poles of the $[n, n+j]$, $j \geqslant -1$, Padé approximant to (2.2) are simple and lie on the positive real axis. Furthermore, the poles of the $[n, n+j]$ Padé approximant interlace with the poles of the $[n+1, n+1+j]$ Padé approximant.*

The error formulae now become:

THEOREM 4.2. *The error made in approximating $f(z)$ with $[n, n+j](z)$, $j \geqslant -1$, is given by*

$$f(z) - [n, n+j](z) = \frac{z^{j+1}}{L_n(z^{-1})} \int_0^\infty \frac{L_n(t)\, d\phi_j(t)}{1 - zt} \tag{4.6}$$

or by

$$f(z) - [n, n+j](z) = \frac{z^{2n+j+1}}{z^n L_n(z^{-1})} \int_0^\infty \frac{t^n L_n(t)\, d\phi_j(t)}{1 - zt}. \tag{4.7}$$

In addition the $[n, n+j]$ Padé approximant is given by

$$[n, n+j](z) = \sum_{l=0}^{j} a_l z^l + \frac{1}{L_n(z^{-1})} \int_0^\infty \frac{L_n(z^{-1}) - L_n(t)}{1 - zt}\, d\phi_j(t), \tag{4.8}$$

where in all of the above L_n is the orthogonal polynomial of degree n with respect to $d\phi_j$.

The analogue of Theorem 3.1 is the following.

THEOREM 4.3. *The $[n, n+j]$ Padé approximant, $j \geqslant -1$, of (2.2) is z^{j+1} times the Gaussian quadrature approximation to (4.1) plus a polynomial of degree j. That is,*

$$\begin{aligned} [n, n+j](z) &= \sum_{l=0}^{j} a_j z^l + z^{j+1} \sum_{k=1}^{n} \frac{\alpha_{nk}}{1 - zx_k} \\ &\doteq \sum_{l=0}^{j} a_j z^l + z^{j+1} \int_0^\infty \frac{d\phi_j}{1 - zt}, \end{aligned} \tag{4.9}$$

where the x_k are the zeroes of L_n, the orthogonal polynomial of degree n with respect to $d\phi_j$, and the α_{nk} are the Gaussian weights.

As corollaries we obtain:

COROLLARY 4.2. *The set $\{[n, n+j](z)\}_{n=1}^{\infty}$, $j \geqslant -1$, is a normal family in $\mathbb{C}\backslash[0, \infty)$ and the residues of $[n, n+j](z)$ are all negative.*

COROLLARY 4.3. *The sequence $\{[n, n+j](z)\}_{n=1}^{\infty}$, $j \geqslant -1$, converges uniformly on compact subsets not intersecting $[0, \infty)$ to*

$$f(z) = \int_0^\infty \frac{d\phi}{1 - zt}$$

if the moments a_m satisfy $a_m = O((2m+1)!\, R^{2m})$ for some $R > 0$.

5. Examples

In this section, we will apply the theory we have developed in previous sections to investigate the rate of convergence of the $[n, n-1]$ Padé approximants in the case

$$f(z) = \int_0^\infty \frac{t^\alpha e^{-t}}{1 - zt}\, dt, \tag{5.1}$$

$\alpha > -1$, $z < 0$. In particular, we will obtain an asymptotic estimate for the error term given in Theorem 2.2, give a table of $[n, n-1]$ for $\alpha = 0$, and compare the table with the known form of $f(z)$.

According to Theorem 2.2, the error term has the form

$$\begin{aligned} E_n(z) &= f(z) - [n, n-1](z) \\ &= \frac{1}{L_n{}^\alpha(z^{-1})} \int_0^\infty \frac{L_n{}^\alpha(t)\, t^\alpha e^{-t}}{1 - zt}\, dt, \end{aligned} \tag{5.2}$$

where $L_n{}^\alpha$ is the nth order generalized Laguerre polynomial. This polynomial can be written in two ways:

$$L_n{}^\alpha(t) = \frac{1}{n!}\, e^t t^{-\alpha} \frac{d^n}{dt^n} (t^{n+\alpha} e^{-t}) \tag{5.3}$$

and

$$L_n{}^\alpha(t) = \frac{\Gamma(\alpha + 1 + n)}{n!\, \Gamma(\alpha + 1)}\, \Phi(-n, \alpha + 1; t), \tag{5.4}$$

where $\Phi(-n, \alpha; t)$ is the confluent hypergeometric function (see Erdelyi [8, Chap. 6 and 10]). Thus, by substituting 5.3 and 5.4 into 5.2 and integrating the resulting expression by parts,

$$E_n = \frac{n!\, \Gamma(\alpha + 1)(-z)^n}{\Gamma(\alpha + 1 + n)\, \Phi(-n, \alpha + 1, z^{-1})} \int_0^\infty \left[\frac{t}{1 - zt}\right]^n \frac{t^\alpha e^{-t}}{1 - zt}\, dt. \tag{5.5}$$

If we now set $\rho = -z^{-1}$ and $\tau = (\rho n)^{-1} t$, (5.5) becomes,

$$E_n = \frac{n!\, \Gamma(\alpha + 1)\, \rho^{\alpha+1} n^\alpha}{\Gamma(\alpha + 1 + n)\, \Phi(-n, \alpha + 1, -\rho)} \int_0^\infty \left[\frac{\tau}{\tau + (1/n)}\right]^n \frac{\tau^\alpha e^{-\rho n \tau}}{\tau + (1/n)}\, d\tau. \tag{5.6}$$

The integral in (5.6) can be put into the form

$$I = \int_0^\infty e^{-ng(\tau)} \frac{\tau^\alpha}{\tau + 1/n}\, d\tau,$$

where $g(\tau) = \rho\tau - \ln(\tau + 1/n) - \ln \tau$. Using standard saddle point methods, this integral has the asymptotic form as $n \to \infty$:

$$I \sim \sqrt{\pi}\, \rho^{(3/4)-\alpha/2} n^{-(\alpha/2)+(1/4)} e^{-2(n\rho)^{1/2}+(1/2)\rho}. \tag{5.7}$$

In addition, $\Phi(-n, \alpha + 1, -\rho)$ has the asymptotic form as $n \to \infty$

$$\Phi \sim \frac{\Gamma(\alpha + 1)}{\sqrt{\pi}} \rho^{-(\alpha/2)-(1/4)} e^{2(n\rho)^{1/2}-(1/2)\rho} \tag{5.8}$$

(see Erdelyi [7, p. 279]). Finally, it is obvious that as $n \to \infty$

$$\Gamma(\alpha + 1 + n)/n! \sim n^{\alpha}. \tag{5.9}$$

Using (5.7), (5.8), (5.9) in (5.6), we have that

$$E_n \sim \pi\rho^{2+\alpha} e^{\rho} n^{-(\alpha/2)+(1/4)} e^{-4(n\rho)^{1/2}} \tag{5.10}$$

as $n \to \infty$.

We now include a numerical example which illustrates the rapid convergence of the $[n, n - 1]$ Padé approximants. The computations were done using the techniques of Section 3.

TABLE I

n	$[n, n-1](-2)$	$[n, n-1](-1)$	$[n, n-1](-0.5)$
2	0.4117647	0.5714285	0.7142857
4	0.4501018	0.5933014	0.7222222
6	0.4579924	0.5957829	0.7226167
8	0.4602080	0.5962146	0.7226519
10	0.4609530	0.5963107	0.7226563
12	0.4612358	0.5963360	0.7226571
	$f(-2) = 0.4614552$	$f(-1) = 0.5963474$	$f(-0.5) = 0.7226572$

The above Table I was computed on a Hewlett–Packard 9830. The function to be approximated is given by (5.1) with $\alpha = 0$. We note that $f(z)$ has the form

$$f(z) = z^{-1} e^{-1/z} Ei(-1/z),$$

where $Ei(-1/z)$ is the exponential integral and is tabulated in many places. We have computed the $[n, n - 1]$ Padé approximants of f for $n = 2, 4, \ldots, 12$ and evaluated this approximation at $z = -2, -1, -0.5$. The exact value of f is given at the bottom of each column. All numbers have been rounded to seven significant digits. We note that as n increases the value $[n, n-1](z)$ increase to the true value of the function. In fact, this behavior on the negative real axis may be proved in general, see, e.g., Baker [3].

We now consider the class of differential equations

$$z^2y'' + (pz - 1)\,y' + qy = 0, \tag{5.11}$$

where $p = q + 2$. We note that $z = 0$ is an irregular singular point of (5.11); despite this we expand y in a formal power series about the origin and observe that the $[n, n+j]$, $j \geqslant -1$, Padé approximants converge to a solution of (5.11). For simplicity we consider the special case of (5.11) when $p = 3$,

$$z^2y'' + (3z - 1)\,y' + y = 0. \tag{5.12}$$

Expanding, we obtain the divergent power series

$$y(z) \sim \sum_{n=0}^{\infty} n!\, z^n. \tag{5.13}$$

Note that this formal series is associated with the Stieltjes integral

$$\int_0^\infty \frac{e^{-t}}{1 - zt}\, dt; \tag{5.14}$$

furthermore, it can be verified that this is indeed a solution to (5.12). If we can compute the $[n, n+j]$, $j \geqslant -1$, Padé approximants to (5.13), then we shall know by Corollary 4.3 that these approximants converge to (5.14) as $n \to \infty$. The remarkable fact is that this summation technique (Padé Approximation) completely recovers the solution (5.14) of (5.12). The other independent solution of (5.11) and (5.12) can be obtained by a formal power series expanded at $z = \infty$.

6. Summary and Remarks

The results of Sections 2–4 indicate the remarkable relationship between Stieltjes series, Padé approximants, and orthogonal polynomials. This leads naturally to the interpretation of the $[n, n+j]$, $j \geqslant -1$, Padé approximant as a quadrature approximation to the integral.

Of course, the arguments used in the previous sections have some immediate generalizations. First, functions like

$$f(z) = \int_0^\infty \frac{e^{-t^2}}{1 - zt^2}\, dt \tag{6.1}$$

may be transformed into a series of Stieltjes by the simple change of variable $u = t^2$. Further, there is really no reason to restrict our integration to the positive real axis. All our arguments hold true for nonnegative measures $d\phi$ on the line with some additional technical assumptions. These are called extended series of Stieltjes.

Algebraically, there is no reason to assume that $d\phi$ is positive. We are presently studying this problem and more results will appear later.

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