COLLOQUIA MATHEMATICA SOCIETATIS JÁNOS BOLYAI
49. ALFRED HAAR MEMORIAL CONFERENCE, BUDAPEST (HUNGARY), 1985.

QUADRATIC AND HIGHER ORDER PADE APPROXIMANTS*

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1. INTRODUCTION

A natural way to generate n-th order algebraic approximants to a function f, analytic at zero, is to consider expressions of the following form

$$(1)\quad E_{m,n}(f:z) := p_{m,n}(z)f^n(z)+p_{m,n-1}(z)f^{n-1}(z)+\dots+p_{m,0}(z) = $$
$$= O(z^{(n+1)(m+1)-1})$$

where the $p_{m,i}$ are polynomials of degree at most m. The n-th order approximant is then a solution of the equation

$$(2)\qquad p_{m,n}(z)y^n + p_{m,n-1}(z)y^{n-1} + \dots + p_{m,0}(z) = 0 .$$

In the case $n = 1$ this leads to the familiar main diagonal Padê approximant. We will call a solution of (2) the (principal) n-th order Padê approximant to f and will call the $p_{m,i}$ the coefficient polynomials. We will call f n-normal if (1) always has a unique solution with $p_{m,n}(z) = z^m + O(z^{m-1})$. The functions we will examine are all n-normal and we will assume throughout that $p_{m,n}$ is normalized so that it has highest coefficient 1.

The hard questions for Padê approximants, like the nature and region of convergence, become harder in this more general setting

* Research supported, in part, by N.S.E.R.C. Some of the material in this paper has been published in [2].

and some new problems arise. For example, (2) has multiple solutions and different branches may be appropriate approximants on different regions. The following results, which are fairly immediate generalizations, indicate some of the similarities to usual Padé approximants.

THEOREM 1. *If* f *is* n*-normal then the* $n+1$ *coefficient sequences,* $\{p_{m,i}\}_{m=0}^{\infty}$ *, all satisfy the same* $n+2$ *term recursion*

$$(3) \qquad 0 = \sum_{k=0}^{n+1} c_{k,m}(z)\, p_{m+k,i}(z)$$

where the $c_{k,m}$ *are polynomials of uniformly bounded degree in* n .

Note that the $c_{k,m}$ depend on m and f , but not on i , so all the coefficient sequences satisfy the same recursion. In the case that the $c_{k,m}$ are also independent of m , which occurs for $(1+z)^{1/(n+1)}$, we have

THEOREM 2. *If the* $c_{k,m}$ *in recursion* (3) *are independent of* m *then* f *is an algebraic function.*

If f is n-normal then the n-th order Padé approximant is locally optimal in the following sense:

THEOREM 3. *If* f *is* n*-normal and*

$$(4) \qquad M_\delta := \min_{\substack{V_i \in \pi_m \\ V_n = z^m + \dots}} \| V_n(z) f^n(z) + V_{n-1}(z) f^{n-1}(z) + \dots V_0(z) \|_{C_\delta}$$

then

$$\lim_{\delta \to 0} \frac{M_\delta}{\| E_{m,n}(f:z) \|_{C_\delta}} = 1 .$$

Here, $\| \ \|_{C_\delta}$ *is the supremum norm on* $C_\delta := \{|z| \le \delta\}$ *and* π_m *denotes the algebraic polynomials of degree at most* m .

These approximations have a considerable history. Hermite analyzed some of the properties of such approximation to exp in [4]. He viewed them as an algebraic extension of the continued fraction. Later Mahler [5] showed how a proof of the transcendence of e and π could be based on this approach and still later [6] proved an irrationality measure for π from this method.

The general Hermite—Padé approximation problem concerning solution of (1), and generalizations, has received considerable attention lately. This material may be accessed through the extensive bibliography in [1]. One can, for example, obtain generalizations of the Montessus de Ballore Theorem. Because the details are, in general, difficult it seems appropriate to offer some very precise special case analysis.

The remainder of this paper is concerned with approximations to exp, log and $x^{1/n}$. The analysis of exp is particularly thorough. The approximations to exp are relatively easy to compute and provide an outstanding method for calculating exp .

2. QUADRATIC PADÉ APPROXIMATION TO exp

We outline the basic formula for the second order Padé approximants to f . The proofs may be pursued in [2].

Let

$$p_m(x) := m! \sum_{j=0}^{m} \frac{c_j x^j}{j!} \tag{5}$$

where

$$c_j := \sum_{k=0}^{m-j} \binom{2m-(k+j)}{m} \binom{m+k}{m} \frac{1}{2^k} .$$

Let

$$(6) \qquad q_m(x) := -2^{m+1} m! \sum_{j=0}^{m} \frac{d_j x^j}{j!}$$

where

$$d_j := (-1)^j \binom{\frac{3m}{2} - \frac{j}{2}}{m} \left(\frac{1+(-1)^{m-j}}{2}\right) .$$

Let

$$(7) \qquad r_m(x) := (-1)^m p_m(-x)$$

and let

$$E_m(x) := p_m(x)e^{-x} + q_m(x)e^{-x} + r_m(x) .$$

The next theorem demonstrates that p_m, q_m and r_m are the coefficient polynomials of the quadratic Padé approximant to exp. It also gives a precise estimate for the error E_m.

THEOREM 4.

a] $E_m(x) := p_m(x)e^{-2x} + q_m(x)e^{-x} + r_m(x) = O(x^{3(m+1)-1})$

where p_m, q_m *and* r_m *are given by* (5), (6) *and* (7) *respectively.*

b] $E_m(x) \sim \dfrac{2^{m+1} m! x^{3m+2} e^{-x}}{(3m+2)!}$.

The asymptotic is uniform on bounded subsets of $\mathbb{C}$. *(As usual,* $a_n \sim b_n$ *means* $\frac{a_n}{b_n} \to 1$ *.)*

PROPOSITION 1. *Let* $D_m := 3m(3m-2)\cdot\ldots\cdot(m+2)$. *Then*

a] $p_m(x) \sim D_m e^{(1-1/\sqrt{3})x}$, b] $q_m(x) \sim (-1)^{m+1} D_m [e^{x/\sqrt{3}} + (-1)^m e^{-x/\sqrt{3}}]$

c] $r_m(x) \sim (-1)^m D_m e^{-(1 - 1/\sqrt{3})x}$.

(The asymptotic is uniform on compact subsets of $\mathbb{C} \setminus \{\pm k\sqrt{3}\pi/2 \mid k = \pm 1, \pm 2, \ldots\}$ *.)*

PROPOSITION 2. *Let*

$$\alpha_m(x) := \frac{-q_m(x) + \sqrt{q_m^2(x) - 4p_m(x)r_m(x)}}{2p_m(x)}$$

where the square root is the principal branch. Then, for odd m *and for* $|x| \le 1$

$$e^{-x} - \alpha_m(x) \sim \frac{2^{m+1} m! x^{3m+2} e^{-x}}{(3m+2)! D_m [e^{x/\sqrt{3}} + e^{-x/\sqrt{3}}]} .$$

(The estimate is uniform on the unit disk.)

This is a remarkably good approximation, α_5 already gives 15 digit accuracy on the unit disk.

Note, for odd m

$$q_m^2(x) - 4p_m(x)r_m(x) \sim D_m^2 [e^{x/\sqrt{3}} + e^{-x/\sqrt{3}}]^2$$

while, for even m

$$q_m^2(x) - 4p_m(x)r_m(x) \sim D_m^2 [e^{x/\sqrt{3}} - e^{-x/\sqrt{3}}]^2 .$$

Thus, while the principal branch of the square root works for the definition of $\alpha_m(x)$ for odd m , we must contend with a branch point near $x = 0$ for even m . Hence, an asymptotic, like Proposition 2, for even m is more complicated. In fact, if

$$\beta_m(x) := \frac{-q_m(x) - \sqrt{q_m^2(x) - 4p_m(x)r_m(x)}}{2p_m(x)}$$

then, for even m ,

$$\alpha_m(t) \sim e^{-t} \quad t \in [-1,0)$$

and

$$\beta_m(t) \sim e^{-t} \quad t \in (0,1] .$$

Let $f_m^*(z) := f_m(z + \frac{1}{3m+2})$. Then, as the following proposition shows, shifted quadratic Padê approximants provided an asymptotically exact minimization on $C_1 := \{|z| \leq 1\}$. Similar results for ordinary rational approximation may be found in [3] and [7].

PROPOSITION 3.

a] $\|p_m^*(z)e^{-2z} + q_m^*(z)e^{-z} + r_m^*(z)\|_{C_1} \sim \frac{2^{m+1}m!}{(3m+2)!}$.

b] *Let*

$$w_m := \min_{\substack{s,t,u \in \pi_m \\ s=z^m+\dots}} \|s(z)e^{-2z} + t(z)e^{-z} + u(z)\|_{C_1} .$$

Then $w_m \sim \frac{2^{m+1}m!}{(3m+2)!}$.

The coefficient polynomials are linked by the following third order differential equations.

PROPOSITION 4.

a] $2mp_{m-1} = p_m''' - 3p_m'' + 2p_m'$

b] $2mq_{m-1} = q_m' - q_m'''$

c] $2mr_{m-1} = r_m''' + 3r_m'' + 2r_m'$.

The recursion for the coefficients is given in the next proposition.

PROPOSITION 5.

a]

$$\mathrm{Det}\begin{bmatrix} p_m(x) & , q_m(x) & , r_m(x) \\ p_{m+1}(x) & , q_{m+1}(x) & , r_{m+1}(x) \\ p_{m+2}(x) & , q_{m+2}(x) & , r_{m+2}(x) \end{bmatrix} = (-1)^{m+1} 9\cdot 2^{m+2}(4+3m)x^{3m+2}$$

b] $\{p_m\}$, $\{q_m\}$, $\{r_m\}$ *and* $\{E_m\}$ *all satisfy the recursion*

$$T_{m+3} = [\tfrac{3}{3m+4}]\Big\{(-2m-14/3)x^3 T_m + [(3m+5)x^2 + (3m+4)(3m+5)(3m+7)]T_{m+1} + xT_{m+2}\Big\}.$$

3. n -TH ORDER PADÊ APPROXIMATION TO log

The next result concerns approximation to $\log z$ at 1.

THEOREM 5. *There exist polynomials* $T_{m,n},\dots,T_{m,0} \in \pi_m$ *so that*

a] $E_{m,n}(z) := T_{m,n}(z)(\log z)^n + \dots + T_{m,0}(z) =$

$= O((z-1)^{(n+1)(m+1)-1})$.

b] *The lead coefficient polynomial in* a] *is given by*

$$T_{m,n}(z) = (-1)^{(n+1)m} \sum_{k=0}^{m} \binom{m}{k}^{n+1} (-1)^{(n+1)k} z^k .$$

c] $|E_{m,n}(x)| \le \frac{n!(m!)^{n+1}}{[(m+1)(n+1)-1]!} (x-1)^{(m+1)(n+1)-1}$ *for* $x \ge 1$.

d] $E_{m,n}(z) = \frac{n!(m!)^{n+1}}{[(m+1)(n+1)-1]!} (z-1)^{(m+1)(n+1)-1} + O((z-1)^{(m+1)(n+1)})$.

PROOF SKETCH. Repeated differentiation and division shows that non-zero expression of type a] cannot have a zero of order greater than $(n+1)(m+1)-1$ at 1 and we deduce the uniqueness of the coefficients in a] up to a multiplicative constant. We observe on differentiating $m+1$ times that $z^{m+1}E_{m,n}(z)^{m+1}$ is a polynomial of degree $n-1$ in $\log z$ with coefficients that are polynomials of degree at most m, and that $z^{m+1}E_{m,n}(z)^{m+1}$ has a zero of order $n(m+1)-1$ at 1. It follows, on normalizing so that the lead coefficient of $T_{m,n}$ is 1, that

$$E_{m,n}(z)^{m+1} = \frac{n \cdot m!}{z^{m+1}} E_{m,n-1}(z)$$

and hence

$$(8) \qquad E_{m,n}(z) = n \int_1^z \frac{(z-t)^m E_{m,n-1}(t)dt}{t^{m+1}} .$$

Also, if $T_{m,n}(z) = a_m z^m + \ldots + a_0$ then one can compute directly that

$$(9) \qquad E_{m,n}(z)^{m+1} = \frac{(-1)^m m! n}{z^{m+1}} \sum_{j=0}^{m} \frac{(-1)^j a_j z^j}{\binom{n}{j}} (\log z)^{n-1} + R(z)$$

where $R(z)$ is of degree $n-2$ in $\log z$.

Part b] follows inductively from (9) while c] and d] follow inductively from (8). The induction starts either at $n = 1$ which is the familiar Padé case, or at $n = 0$ in which case one has

$$z^{m+1}E_{m,1}(z)^{m+1} = m!(z-1)^m .$$

(Similar estimates may be found in [5] and [6].) □

For $n = 2$ we have

$$(10) \quad E_m(x) := t_m(x)(\log x)^2 + u_m(x)(\log x) + v_m(x) = O((x-1)^{3(m+1)-1})$$

where

$$t_m(x) := (-1)^m \sum_{k=0}^{m} \binom{m}{k}^3 (-x)^k .$$

One can derive the following recursion for $\{t_m\}$, $\{u_m\}$ and $\{v_m\}$.

PROPOSITION 6. *The sequences* $\{t_m\}$, $\{u_m\}$, $\{v_m\}$ *and* $\{E_m\}$, *as defined above, all satisfy the recursion*

$$T_{m+3} = a(x-1)^3 T_m - (bx^2 + cx + d)T_{m+1} + e(x-1)T_{m+2} \tag{11}$$

where

$$a = (3m+7)(m+1)^2/D ,$$
$$b = d = (3m+5)(3m^2 + 11m + 9)/D ,$$
$$c = (3m+5)(21m^2 + 77m + 66)/D ,$$
$$e = (9m^3 + 57m^2 + 116m + 74)/D$$

and

$$D = (3m+4)(m+3)^2 .$$

The initial values are

$$t_0 = 1 \; ; \; t_1 = x-1 \; ; \; t_2 = x^2 - 8x + 1 ,$$
$$u_0 = 0 \; ; \; u_1 = -6x - 6 \; ; \; u_2 = -9x^2 + 9 ,$$
$$v_0 = 0 \; ; \; v_1 = -12x - 12 \; ; \; v_2 = 24x^2 - 48x + 24 .$$

Note that at $x = 1$, (11) *reduces to*

$$T_{m+3}(1) = -(bx^2 + cx + d)T_{m+1}(1)$$

and we can deduce an identity of Dixon's, namely

$$t_{2m}(1) = \sum_{k=0}^{2m} \binom{2m}{k}^3 (-1)^k = \frac{(3m)!}{(m!)^3} \cdot (-1)^m .$$

The proof of Proposition 6 is entirely mechanical. Once one knows the general form of the recursion (11) and also a specific solution, namely $\{T_m\}$, one can solve for a, b, c, d and e as rational functions of m by inserting the first few coefficients of T_m, T_{m+1}, T_{m+2} and T_{m+3} in (11). This was done with the aid of the symbolic manipulation package Maple.

4. (n-1) -ST ORDER PADÉ APPROXIMATIONS TO $x^{1/n}$

We write

$$(x^{1/n} - 1)^{(m+1)n-1} = p_{m,n-1}(x)x^{\frac{n-1}{n}} + p_{m,n-2}(x)x^{\frac{n-2}{n}} + \dots + p_{m,0}(x)$$

where

$$p_{m,n-i}(x) = \sum_{k=0}^{m} \binom{(m+1)n-1}{(k+1)n-i} x^k (-1)^{(m-k)n+i-1}$$

and observe that we have constructed the normal $(n-1)$ -st order Padé approximant to $x^{1/n}$ at $x = 1$.

For fixed n, $\{p_{m,n-i}\}_{m=0}^{\infty}$ satisfies a recursion

$$p_{m+n,n-i}(x) = \sum_{k=0}^{n-1} c_{k,n}(x) p_{m+k,n-i}(x)$$

where $c_{k,n}$ is independent of both m and i. The coefficients of the first few recursions are as follows:

$n = 2$:

$c_{0,2}(x) = -(x-1)^2$

$c_{1,2}(x) = 2x + 2$

$n = 3$:

$c_{0,3}(x) = (x-1)^3$

$c_{1,3}(x) = -3x^2 - 21x - 3$

$c_{2,3}(x) = 3x - 3$

$n = 4$:

$c_{0,4}(x) = -(x-1)^4$

$c_{1,4}(x) = 4x^3 + 124x^2 + 124x + 4$

$c_{2,4}(x) = -6x^2 + 124x - 6$

$c_{3,4}(x) = 4x + 4$

$n = 5$:

$c_{0,5}(x) = (x-1)^5$

$c_{1,5}(x) = -5x^4 - 605x^3 - 1905x^2 - 605x - 5$

$c_{2,5}(x) = 10x^3 - 1905x^2 + 1905x - 10$

$c_{3,5}(x) = -10x^2 - 605x - 10$

$c_{4,5}(x) = 5x - 5$

$n = 6$:

$c_{0,6}(x) = -(x-1)^6$

$c_{1,6}(x) = 6x^5 + 2736x^4 + 20586x^3 + 20586x^2 + 2736x + 6$

$c_{2,6}(x) = -15x^4 + 20586x^3 - 131727x^2 + 20586x - 15$

$c_{3,6}(x) = 20x^3 + 20586x^2 + 20586x + 20$

$c_{4,6}(x) = -15x^2 + 2736x - 15$

$c_{5,6}(x) = 6x + 6$.

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