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SOME NUMERICAL RESULTS ON THE CONVERGENCE OF INTEGRAL APPROXIMANTS

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ABSTRACT. I review some work in which integral approximants (a special case of Hermite-Padé approximants) based on second-order, inhomogeneous, linear differential equations are applied to a series of test functions. Previous theoretical analysis has pointed out various function classes as particularly appropriate for study. Some existing theorems are illustrated and the numerical results reported give an indication of the general rates of convergence to be expected. In the comparison of the rates of convergence between "diagonal" and "horizontal" types of approximants, the "diagonal" type is usually superior (but not always) to the "horizontal" type. Comparison is made with some other methods applied to some of the same test series. Quite good convergence is obtained with the integral approximants for a diverse set of test functions; however, as with any such general type of series summation (or approximate analytic continuation) method, a moderately large number of series coefficients is required.

Integral Approximants are a special case of Hermite-Padé approximants of the Latin type. They are defined as follows: Let us be given a formal power series

$$f(z) = \sum_{j=0}^{\infty} f_j z^j. \tag{1}$$

Next define the polynomials $Q_j^{(\overrightarrow{q})}(z),\ j = 0, \ldots, m$, and $P^{(\overrightarrow{q})}(z)$ by the accuracy through order principal from

$$\sum_{j=0}^{m} Q_j^{(\overrightarrow{q})}(z) f^{(j)}(z) + P^{(\overrightarrow{q})}(z) = O(z^{(s+1)}), \tag{2}$$

where the degree of $Q_j^{(\overrightarrow{q})}$ is q_j, that of P is p, and

$$\overrightarrow{q} = (q_1, q_2, \ldots, q_m, p), \qquad s = m + p - 1 + \sum_{i=0}^{m} q_i. \tag{3}$$

These $(\overrightarrow{Q}, P)$ always exist [**7**] as there is one more unknown than there are equations and also $\overrightarrow{Q}$ is never identically zero.

Now, in order to define the integral approximant (the integral curve for a differential equation), one solves

$$\sum_{j=0}^{m} Q_j^{(\overrightarrow{q})}(z) y^{(j)}(z) + P^{(\overrightarrow{q})} = 0, \tag{4}$$

subject to

$$y(0) = f(0),\ y'(0) = f'(0), \ldots, y^{(m-1)}(0) = f^{(m-1)}(0). \tag{5}$$

If $Q_m^{(\overrightarrow{q})}(0) \neq 0$, then this solution exists. If $Q_m^{(\overrightarrow{q})}(0) = 0$, however, then there may be a restriction on the initial conditions required to achieve a regular solution.

The monodromic dimension of a functional element [**2**] is the number of linearly independent coverings of the complex plane generated by the associated monogenic analytic function. As the solution of an m-th order homogeneous ordinary differential equation ODE has m linearly independent solutions, therefore the monodromic dimension of the integral curve is less than or equal to m. It could be less than m, if, for some case, not all the solutions were connected by analytic continuation with one starting from a particular boundary condition.

The final aim in this paper is to consider some practical questions. For example, is there convergence of

$$y^{(\overrightarrow{q})}(z) \to f(z) \quad \text{as } |\overrightarrow{q}| \to \infty? \tag{6}$$

If the answer to that question is yes, then what sequence of $\overrightarrow{q}_k$ of integral approximants should be chosen for the best results? Does this sequence depend on $f(z)$ and, if so, how? Of course, no complete answers are yet known.

As background I now review a little bit of what is known about the case $m = 0$, that is, Padé approximants, in this regard. I will not try to be either complete or even very precise, as this review is meant only for motivation in the subsequent numerical studies reported.

For horizontal sequences $[L/m], L \to \infty$ with m fixed, we have the theorem of Montessus de Ballore [**1, 4**] which implies convergence in the largest disk with exactly m poles, counting multiplicity, and no other singularities. The rate of convergence is geometric (with a small circle around each pole excluded) and the convergence is pointwise. For diagonal sequences, $[L/M], M \to \infty, L/M \to \lambda, 0 < \lambda < \infty$, we have Pomerenke's theorem [**1, 4**], which implies that, in an appropriately cut complex-plane, except for a set of zero capacity, convergence is obtained for reasonable functions. The question of pointwise convergence of a subsequence is not yet settled.

The standard notation for the solution of (4)–(5) is $[p/q_0; \dots ; q_m]$, where the q_j's are defined at (2). Now, for integral approximants, $m > 0$, there are more plausible choices for sequences to study than just "horizontal" and "diagonal" sequences. For example, for $[L/M; N; P]$, we could have $L \to \infty$ with M, N, P fixed, or $L, M \to \infty$ together or $L, M \to \infty$ with $L\mathbf{M} \to \infty$ (or $LM \to 0$) while N, P are fixed. We could have $L, M, N \to \infty$ at various rates with P fixed. Also, $L, N \to \infty$ with P, M fixed, etc.

Some results have been proven for "horizontal" sequences.

Theorem (Baker-Lubinsky). *Let $f(z)$ be analytic at $z = 0$ and a meromorphic function in $|z| < R, 0 < R \le \infty$ with l distinct poles, $z_1, \dots , z_l$ having multiplicies $p_1, \dots , p_l$. Define*

$$
\begin{gathered}
p = \sum_{j+1}^{l} p_j, \qquad S_1(z) = \prod_{j=1}^{l}(z - z_j), \qquad S(z) = \prod_{j=1}^{l}(z - z_J)^{p_j} \\
(\overrightarrow{q}) = (\overrightarrow{m}, p), \qquad M = \sum_{j=0}^{m}(q_j + 1) - 1 = p + ml.
\end{gathered} \tag{7}
$$

Then, for the sequence

$$\overrightarrow{m} = (p - 1, l - 1, \dots , l - 1, -1, \dots , -1, tl), \tag{8}$$

where there are $m - t \ge 0$ entries, $(l - 1)$, and $t - 1 \ge 0$ entries, (-1)*, in* (8)*, it follows that*

$$\limsup_{k\to\infty} ||[p/q_0; \dots ; q_m] - f(z)|| \begin{matrix} 1/p \\ \mathcal{K} \end{matrix} < \frac{||z||_{\mathcal{K}}}{R} \tag{9}$$

for $\mathcal{K}$ any compact subset of $|z| < R$ with no poles of $f(z)$. In addition $Q^{(\overrightarrow{q})}_{m}(z) \to [S_1(z)]^t$.

The next results concern the separation property and are due to Baker et al. [**8**]. This property seems to play the role for integral approximants that the class of meromorphic functions does for Padé approximants.

Definition. If $f(z)$, possibly multiform, can be written as $f(z) = f_i(z) + f_o(z)$ for a disk $\mathcal{D} = \{z|\,|z| \le R\}$ and $f_o(z)$ is analytic if $z \in \mathcal{D}$ and $f_i(z)$ is analytic on every analytic continuation to all $z \notin \mathcal{D}$ in the finite complex plane, then $f(z)$ has the *separation property with respect to* $\mathcal{D}$.

From this property, Baker et al. [**8**] have been able to prove the following theorem.

Theorem (Separation Property). *Let $f(z)$ have the separation property with respect to a disk $\mathcal{D}$, a finite number of singular points $a_i(|a_i| > 0, \forall i)$ in the interior of $\mathcal{D}$. Assume that all these singular points and the point at ∞ for $f_i(z)$ are of finite order, and let $f_i(z)$ be of exact monodromic dimension m. Then* (i) *there exists essentially unique polynomials $A_j(z)$ with $A_m(z)$ of minimum degree such that*

$$\sum_{j=0}^{m} A_j(z) f^{(j)}(z) = \phi, \tag{10}$$

where ϕ is analytic in $\mathcal{D}$, and (ii) *if q_j is the degree of A_j for $j = 0, \dots, m$, furthermore,*

$$\lim_{L \in \infty} [L/q_0; \dots ; q_m] = f(z) \tag{11}$$

uniformly on simply connected compact subsets of $\mathcal{D}\backslash\{\alpha_\kappa\}$ which contain the origin.

Baker and Graves-Morris [**5**] have obtained accurate estimates of the rate of convergence at the singularity nearest the origin. Suppose that in $|z| \leq \rho, \rho > 1$, the functions $G(z)$ and $H(z)$ are analytic and we define $f(z)$ by

$$(1-z)f'(z) + G(z)f(z) = H(z), \tag{12}$$

with $f(0)$ given. Then, by the standard theory of ODE, $f(z)$ has a singularity at $z = 1$ like

$$f(z) = A(z)(1-z)^{-\gamma} + B(z), \qquad \gamma = -G(1), \tag{13}$$

provided that γ is not an integer. $A(z)$ and $B(z)$ are analytic in the neighborhood of $z = 1$ generally and in $\{z|\,|z| < \rho\}$. They have shown, for the case $[L/M; 1]$ with M fixed and $L \to \infty$, that

$$\begin{aligned} z_s^{(L)} &= 1 + O(L^{-M-2}, \\ \gamma^{(L)} &= \gamma + O(L^{-M-1}). \end{aligned} \tag{14}$$

Baker and Graves-Morris [**5**] have also considered the case of a second order ODE. Here $K(z)$ and $H(Z)$ are analytic in $|z| < \rho, \rho > 1$, and $f(z)$ is defined by

$$(1-z)^2 f''(z) + (1-z)G_0 f\prime(z) + K(z)f(z) = H(z), \tag{15}$$

where now $f(0), f'(0)$ are given. They assume that the corresponding indicial equation,

$$\nu^2 + (G_0 + 1)\nu + K(1) = 0, \tag{16}$$

has two roots γ, θ and that (neither an integer) $\mathrm{Re}\gamma > \mathrm{Re}\theta > \mathrm{Re}\gamma - 1$. The standard theory of ODE leads to the solution of (14),

$$f(z) = A(z)(1-z)(1-z)^{-\gamma} + B(z)(1-z)^{-\theta} + C(z), \tag{17}$$

where $A(z), B(z)$ and $C(z)$ are analytic in $\{z|\,|z| < \rho\}$. They call this a confluent singularity because they are two “independent” singularities at the same place. They consider the sequence $[L/M; 1; 2]$ with M fixed and $L \to \infty$. The dominant error in the estimation of the behavior in the vicinity of the singular point, $z_s = 1$ arises from the equation for z_s, e.g., for $M \geq 2$,

$$z_s^2 - [2 + O(L^{-M-1})]Z_s + [1 + O(L^{\theta-\gamma-M-2})] = 0, \tag{18}$$

which simply implies

$$z_s = 1 + O(L^{-M-1}) \pm O(L^{-\frac{1}{2}(M+1)}). \tag{19}$$

Thus $\frac{1}{2}(z_s^+ + z_s^-)$ gives the asymptotically best estimate of $z_s = 1$, rather than either z_s^+ or z_s^-.

For the case of "diagonal" sequences we have the theorems of Baker [**3**] and Stahl [**12**]. Here, by "diagonal," is meant the $[L/M; \ldots; N]$ sequences where $\lim_{L\to\infty} M/L = \cdots = \lim_{L\to\infty} N/L = 1$. These theorems imply geometric convergence at regular points and where a singularity can be exactly represented by the approximant. The region is the suitably cut complex plane and its pendant, identically-cut, higher Riemann sheets. The cut structure is such as to leave a region in which the function can be identically represented by the approximant. The theorems are silent on the rate of convergence at singularities which cannot be exactly represented or on branch cuts.

Next I discuss a few of the practical problems that confront approximation at a confluent singularity. I have already touched on this question in reviewing the work of Baker and Graves-Morris [**5**]. Specifically, if there are m singularities at a single point (say $z = 1$ for convenience), as in (17) with two such for example, the most likely approximation obtained with an integral approximant is a cluster of m isolated singularities near this singular point. Their singular exponents do not directly yield the singular exponents of the confluent singularities. Baker et al. [**8**] have suggested a method to deal with this problem. The theorems of Baker [**3**] and Stahl [**12**] imply, when the approximation is good, that the approximant converges well, away from the singular point, and that if one were to integrate out along the real axis to a point r $[0 < r < 1, \max(0, 2-\rho) < r$, in the example of (15)] and then to encircle the singular point n times, returning to a point on a higher Riemann sheet each time which lifts onto r, one could expect that the integral approximant would yield a good approximation to

$$f_n(z) = e^{-2\pi i n\gamma}(1-z)^{-\gamma}A(z) + e^{-2\pi i n\theta}(1-z)^{-\theta}B(z) + C(z), \tag{20}$$

where the example of (17) is used here and subsequently for ease of exposition. At this point monodromy group ideas are used to proceed further. Since there are at most three linearly independent solutions to (15), and one of them is basically an "analytic background term" coming from the inhomogeneous term, we therefore write

$$\left\{\begin{matrix} f_{1+j} \\ f_{2+j} \\ f_{3+j} \end{matrix}\right\} = \mathbf{M}^{\,j+1} \left\{\begin{matrix} f_0 \\ f_1 \\ f_2 \end{matrix}\right\}, \qquad j = 0, 1, 2. \tag{21}$$

The monodromy matrix $\mathbf{M}$ has eigenvalues of $e^{-2\pi i\gamma}, e^{-2\pi i\theta}$, and 1, as can be deduced from (20). These eigenvalues are directly related to γ and θ. The last eigenvalue corresponds to the analytic background term $C(z)$ in (16). The equations for the elements of $\mathbf{M}$ are easily given from (21) as

$$f_{i+j} = \sum_{k=1}^{3} M_{ik} f_{k+j-1}, \quad i = 1, 2, 3, \qquad j = 0, 1, 2, \tag{22}$$

which can be solved in general for the first two rows as

$$\mathbf{M} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ M_{31} & M_{32} & M_{33} \end{pmatrix}. \tag{23}$$

Baker et al. [**8**] call this the contour method of estimation for the confluent singularity exponents. It will be noticed that the eigenvalues of the monodromy matrix are insensitive to the integer part of γ and θ. Baker et al. [**8**] give an approximate method which seems sufficient to resolve this ambiguity.

In the following tables of numerical results, I tabulate the quantity

$$\epsilon = -\log_{10}\left(\frac{|t - t_{exact}|}{|t_{exact}|}\right), \tag{24}$$

i.e., the number of decimal places of agreement in the quantity being considered. The numerical data reported here come from Guttmann [**10**], Hunter and Baker [**11**], and Baker et al. [**8**].

As a partial check of their computer codes Guttmann [**10**] and Baker et al. [**8**] have computed the $[L/M; N; P]$ (second-order, inhomogeneous ODE) to the test function

$$A(z) = (1 - z)^{-1.5} + e^{-x}. \tag{25}$$

They found that it satisfies

$$(26) \quad (1-z)\left(\frac{5}{2}-z\right)A'' - \left(\frac{11}{4}+2z-z^2\right)A' + \left(\frac{3}{2}z-\frac{21}{4}\right)A = 0$$

as can be verified directly.

The test function

$$(27) \qquad M(z) = \frac{\tan\sqrt{z}}{\sqrt{z}},$$

has simple poles at $z_n = (n+\frac{1}{2})^2\pi^2$ and illustrates the theorem of Baker and Lubinsky quoted above. Numerical results are shown in Table 1. The column headed n lists the number of coefficients used, here and in subsequent tables.

TABLE 1. Results for the test function M of (27).

n	z_1	γ_1	z_1	γ_1
	$[L/0;0;1]$		diagonal	
18	12.5	11.0	23	21.4
n	z_2	γ_2	z_2	γ_2
	$[L/1;1;2]$		diagonal	
18	3.6	2.2	7.5	6.0
24	5.4	3.9	8.4	6.9

Of course it is not for meromorphic functions that we are studying the integral approximants. I therefore next consider two test functions which have monodromy dimension $m = 2$ with an analytic background term and have the separability property

$$(28) \qquad \begin{aligned} K(z) &= (1-z)^{-1.5} + \left(1+\frac{4}{5}z\right)^{-1.25} + e^{-z}, \\ U(z) &= (1-z)^{-\frac{7}{4}} + (1-z)^{-\frac{3}{4}} + \left(1+\frac{1}{2}z\right)^{-\frac{5}{4}} + e^{-z}. \end{aligned}$$

In function U the second term is just an analytic correction to the first term and not an independent singularity in the sense of the monodromy group. Even so we expect a double zero in the coefficient of U'' as can be seen from a simple calculation. Some results are listed in Table 2.

TABLE 2. Results for test functions K and U of (28).

	n	z_1	γ_1	z_1	γ_1
		$[L/2;2;3]$		diagonal	
K	18	7.7	5.1	6.0	4.6
	28	14.2	12.5	11.6	9.7
		$[L/1;2;3]$		diagonal	
U	18	6.5	5.0	8.3	6.2
	28	16.2	14.5	12.6	10.7

	n	z_2	γ_2	z_2	γ_2
		$[L/2;2;3]$		diagonal	
K	18	4.0	2.4	3.0	1.1
	28	12.5	10.8	9.0	7.0
	40	21.9	20.9	14.0	11.8
		$[L/1;2;3]$		diagonal	
U	18	2.2	1.3	1.5	0.3
	28	5.2	3.5	3.9	2.2
	40	5.8	3.9	8.0	5.6

For test function K a number of other methods have been tried. They are the standard d log Padé method [**4**] which I will denote by P, the generalized approximant method [**2**] denoted by G, the ratio method [**9**] denoted by R, integral approximants based on a first-order ODEdenoted by $IA1$ [**11**], and the recurrence relation method denoted by RR [**10**]. Some results are listed in Table 3.

TABLE 3. Other results for test function K.

n	R	P	G	$IA1$	RR
		Singular-Point Estimates			
10	1.1	0.7		3.4	2.4
15	1.7	3.0		5.2	3.2
20	2.0	3.9	6.5	6.9	5.3
		Singular-Point Exponent Estimates			
10	0.1	0.1		1.7	1.2
15	0.5	1.7		3.8	1.9
20	0.8	2.3	5.5	5.5	3.4

It can be seen by a comparison of Tables 2 and 3 that in this case the method of integral approximants based on second order ODE is comparable in accuracy to the best of the other methods.

Now I report on test series which have a global monodromy dimension of three, which exceeds that which could be approximated by the solution to a second order differential equation and so cannot be exactly represented by the integral approximants which we are studying. The test functions are

(29)
$$D(z) = (1-z)^{-1.5} + \left(1+\frac{1}{4}z^2\right)^{-1.25} + \left(1+\frac{15}{112}z-\frac{1}{4}z^2\right)^{-1.25}$$

$$E(z) = (1-z)^{-1.5}(1+\frac{1}{2}z) + \left(1+\frac{1}{4}z^2\right)^{-1.25} + \left(1+\frac{15}{112}z-\frac{1}{4}z^2\right)^{-1.25}$$

$$H^*(z) = (1-z)^{-1.5} + \left(1+\frac{1}{2}z\right)^{-1.5} + \left(\frac{2(1-z)(2-z)^6}{(2-z)^7-z^7}\right)^{1.25}.$$

The test functions D and H^* are separable in the disk containing the closest singularity to the origin and E is not. By the results of Baker and Graves-Morris [**3**] the horizontal sequences should converge at $z=1$ to give estimates of z_{singular} and of $\gamma = 1.5$. Numerical results are quoted in Table 4. At the second singularity, fair convergence is observed for the test functions D and E and poor convergence for H^*. For test functions D and E there is also a similar set of results from other methods just as I reported above for test function K. They are reported in Table 5.

Again, for the test functions presented in Tables 4 and 5, a comparison shows, as it did for test function K, that the method we are considering is quite comparable with the best of the other methods reported.

Finally, I report numerical results on the convergence of integral approximants based on a second order ODE at a confluent singularity.

TABLE 4. Results for test functions D, E and H^*.

	n	z_1	γ_1	z_1	γ_1
		$[L/1;2;3]$		diagonal	
D	18	2.8	1.5	4.3	3.3
	28	5.7	4.0	7.0	5.2
	40	7.9	6.2	12.0	9.7
	50	11.1	9.4	13.3	10.9
		$[L/4;4;5]$		diagonal	
E	18	3.5	2.1	4.0	2.6
	28	6.5	4.7	6.7	5.0
	40	8.6	6.6	10.4	8.3
	50	9.6	7.2	15.2	12.8
		$[L/4;4;5]$		diagonal	
H^*	18	1.9	0.9	1.9	1.0
	28	2.2	0.8	3.0	1.7
	40	3.1	1.3	5.9	4.1

TABLE 5. Other results for test functions D and E.

	n	R	P	G	$IA1$	RR
			Singular-Point Estimates			
D	10	1.7	1.9		2.1	
	15	2.6	2.2		4.0	2.0
	20	3.6	3.5	5.4	5.3	4.0
E	10	1.6	1.3		2.7	
	15	2.4	2.5		3.6	2.0
	20	3.0	3.7	3.8	4.8	3.6
			Singular-Point Exponent Estimates			
D	10	0.8	0.7		1.7	
	15	1.4	1.0		2.2	0.8
	20	2.0	1.9	4.3	3.6	2.4
E	10	0.7	0.4		2.3	
	15	1.3	1.4		2.3	0.7
	20	1.7	2.2	1.7	3.3	2.1

Two test functions are used. They are

$$
\begin{aligned}
V(z) &= (1-z)^{-\frac{7}{4}} + (1-z)^{-\frac{5}{4}} + \left(\frac{1-\frac{1}{3}z}{1+\frac{1}{3}z}\right)^{\frac{1}{2}}, \\
W(z) &= \left(\frac{1-z}{1+\frac{1}{2}z}\right)^{-\frac{7}{4}} + \left(\frac{1-z}{1+z}\right)^{-\frac{7}{4}} + \left(\frac{1+\frac{1}{5}z}{1-\frac{1}{3}z}\right)^{\frac{1}{2}}.
\end{aligned} \tag{30}
$$

Both of these test functions have monodromy dimension three. The test function V is separable with respect to the disk enclosing the nearest singularity to the origin, and W is not. Again Baker and Graves-Morris [**3**] have proven convergence of a horizontal sequence at $z = 1$ for $z_{\text{singular}}, \gamma$ and θ. The results are reported in Table 6.

TABLE 6. Results for test functions V and W.

	n	z_1	γ_1	γ_2	z_1	γ_1	γ_2
		$[L/0;1;2]$			diagonal		
V	18	3.4	0.0	0.0	3.7	1.6	0.9
	28	3.7	2.5	2.3	4.2	3.3	2.0
	40	8.0	7.4	7.0	6.5	5.0	3.8
	50	12.4	11.6	11.2	8.1	6.6	5.3
w	18	3.5	0.0	0.0	3.5	0.0	0.0
	28	3.8	2.9	2.3	4.1	4.5	2.4
	40	4.4	2.7	2.0	5.3	5.5	4.0
	50	7.8	6.6	5.7	8.6	7.1	5.9

The general conclusions that I draw from these numerical experiments are:

(1) Integral approximants can be highly successful in the analysis of power series for quite complicated functions.

(2) Usually diagonal sequences converge faster than horizontal ones.

(3) The contour method of estimating confluent singularities often gives better results than the approximate formula, but usually the difference is not great [**8**].

(4) There is an advantage in increasing the complexity of the approximant in order to match the structure of the function being approximated, but the use of a more complex approximant than that appropriate to the function is not likely to be advantageous because of the higher cost in terms of the number of series coefficients required to determine it.

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