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The analysis of double power series using Canterbury approximants

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Abstract. The recent scheme of approximants formed from double power series and proposed by Chisholm is examined in relation to known functions containing simple singularities of the form $(x - x_s(y))^{-\gamma}$, in cases where $x_s(y)$ is linear. Attention is focused on the usefulness of these approximants in determining sequences of approximations to the locus of singularities $x_s(y)$, and the exponent γ.

1. Introduction

Within the last two years or so, a number of authors have attempted to generalize the rational approximation scheme known as the Padé approximant to approximation schemes for functions of two or more variables defined through a many-variable power series expansion (Chisholm 1973, Chisholm and McEwan 1974, Lutterodt 1974, Watson 1974). The many-variable approximants of Chisholm and McEwan possess many of the algebraic properties of Padé approximants, which have been so very successful and well tested on many problems in theoretical physics (Baker and Gammel 1970, Gaunt and Guttmann 1974, Hunter and Baker 1973). The purpose of this paper and its companion paper (Wood and Fox 1975, hereafter referred to as II) is to examine in numerical detail the scheme of two-variable approximants which has been developed by the Canterbury group.

The applications of Canterbury approximants (CA) which are reported in II are to a selection of double power series expansions which occur in the field of critical phenomena; our purpose here is to review the performance of the CA scheme on a variety of *known* two-variable functions. Of particular interest is the ability of the CA scheme to determine such analytic features as the locus of singularities in the x–y plane, and the residues of these singularities, which correspond to the locus of critical points, and the values of the critical exponents in II. For these purposes we have examined a variety of two-variable functions which are generalizations of the test functions used by Hunter and Baker (1973) in their recent review of the Padé approximant scheme for use in critical phenomena. Applications of CA in potential scattering theory have been given by Graves-Morris and Samwell (1975). The test functions we include here are:

(i) functions with one set of singularities:

$$(1-2x+y)^{-\gamma}+\mathrm{e}^{-2x+y} \qquad (1a)$$

$$(1-2x+y)^{-\gamma}+\mathrm{e}^{x-2y}; \qquad (1b)$$

and

(ii) functions with two sets of singularities:

$$(1-x-\tfrac{1}{2}y)^{-3/2}(1-2x-\tfrac{1}{5}y)^{-1/2}+e^{-x-2y} \tag{2a}$$

$$(1-x-\tfrac{1}{5}y)^{-3/2}(1-\tfrac{1}{2}x-\tfrac{1}{2}y)^{-5/4}+e^{-x-2y} \tag{2b}$$

$$(1-x-\tfrac{1}{2}y)^{-3/2}(1-2x+\tfrac{1}{5}y)^{1/2}+e^{-x-2y} \tag{2c}$$

$$(1-x)^{-3/2}(1-\tfrac{1}{2}y)^{-1/2}+e^{-x-2y}. \tag{2d}$$

The Canterbury approximant $\mathrm{CA}(n_1, n_2, m_1, m_2)$ is defined from the double power series

$$f(x,y) = \sum_{\alpha,\beta} c_{\alpha\beta}x^{\alpha}y^{\beta} \tag{3}$$

and takes the form

$$\mathrm{CA}(n_1, n_2, m_1, m_2) = \frac{\sum_{\mu=0}^{m_1}\sum_{\nu=0}^{m_2} a_{\mu\nu}x^{\mu}y^{\nu}}{\sum_{\sigma=0}^{n_1}\sum_{\tau=0}^{n_2} b_{\sigma\tau}x^{\sigma}y^{\tau}} \tag{4}$$

such that on expansion the approximant reproduces the expansion of $f(x, y)$ to as high an order as possible (Chisholm and McEwan 1974, Chisholm 1973). The approximant in (4) is known as the general off-diagonal case (GOD) (Hughes-Jones 1973), while the special case $n_1 = n_2 = n$, $m_1 = m_2 = m$, which is used here and in II, is known as the simple off-diagonal case (SOD) and is denoted by $\mathrm{CA}(n, m)$. The original method of forming a sufficient number of linear equations for the coefficient sets $\{\underline{a}\}$ and $\{\underline{b}\}$ (Chisholm 1973) for the $\mathrm{CA}(n, n)$ was to create n linear conditions (symmetrical in x and y) by equating the sums of coefficients of the n pairs of terms

$$x^{\gamma}y^{2n+1-\gamma},\ x^{2n+1-\gamma}y^{\gamma} \qquad (\gamma = 1, 2, \ldots n).$$

For the SOD case $\mathrm{CA}(n, m)$ this scheme of symmetrizing the equations is described by Graves-Morris *et al* (1974); it is this scheme which is used here and in II. Under this algorithm the approximants in (4) are not invariant to a change of scale in either of the variables. Two alternative schemes have recently been suggested by Hughes-Jones and Graves-Morris (1974) and by Hughes-Jones and Chisholm (1975); the latter algorithm establishes the property of scale covariance for the approximants in (4), which is also a property of the Padé approximant. A comparison of all three algorithms, together with a computer subroutine for the GOD in (4), has been given by Graves-Morris and Roberts (1975a, b).

For functions of the form

$$\sum_{i=1}^{N} c_i(1+a_ix+b_iy)^{-1} \tag{5}$$

all the approximants $\mathrm{CA}(n, n)$ $(n \geqslant N)$ are exact; thus for functions which have lines of branch-point singularities with the dominant form

$$\sim (x - x_s(y))^{-\gamma} \tag{6}$$

in the region of the singularities $x_s(y)$, we adopt the customary procedure of converting the function into its logarithmic partial derivatives and we determine the CA sequences to the expansions of the latter. The CA sequences show some sensitivity to the exponential functions in (1) and (2), these functions being included to mask the singularity, and the coefficients of x and y in the exponentials can substantially affect the range over which good convergence is achieved, and also the rate of convergence. Thus from the viewpoint of applications, the CA sequences may be substantially affected by the function $A(x, y)$ in an asymptotic form,

$$f(x, y) \sim A(x, y)(x - x_s(y))^{-\gamma}. \tag{7}$$

This effect may be illustrated by the wider-ranging fits obtained for the anisotropic Heisenberg models than for the second-neighbour Ising model in II.

In §§ 2 and 3 we report on the sequences of approximations to the locus of singularities $x_s(y)$ and to the values of the exponents γ in functions (1*a*)–(2*d*).

It is commonly the case in critical phenomena series expansions that the coefficient matrix $C(c_{\alpha\beta})$ is triangular in form; thus the function has an expansion in the form

$$f(x, y) = 1 + \sum_{l=1}^{\infty} P_l(y)x^l \tag{8}$$

where $P_l(y)$ is a polynomial of degree l. An existence condition on the CA is that the Padé approximants to $f(0, y)$ and $f(x, 0)$ both exist, which fails in (8). To overcome this difficulty a rotation of $\pi/4$ in the x–y plane can be made which fills up the coefficient matrix (Wood and Griffiths 1974). The approximants used here are not covariant under such transformations; hence to assess the reliability of this additional procedure we have compared the CA sequences of a given function with and without the use of the rotation. If the rotation is used, the approximant obtained must be transformed back again into x, y before evaluating the singularities and residues.

2. Functions with one set of singularities: $(x - x_s(y))^{-\gamma}$

We have examined the sequences CA$(n, n \pm j)$ $(j = 0, +1)$ to the functions (1*a*) and (1*b*) with $\gamma = \frac{1}{10}, \frac{1}{2}$ and $\frac{3}{2}$. As a typical example of these calculations we include here the diagonal $(j = 0)$ sequence $n = 3, 5, 7, 9$ for the case $\gamma = \frac{3}{2}$. These results are displayed in tables 1 and 2, which list the errors in the estimates of the singularities $x_s(y)$ and the exponent γ respectively, on the interval $y = (1, -1)$. Each function has been examined using the rotation operation $(\theta = \pi/4)$ and compared with the corresponding untransformed approximants $(\theta = 0)$.

The first observation is that the diagonal sequence is clearly converging well in the case of (1*a*), with very acceptable results over the whole range $[1, -1]$ being obtained at CA(9, 9). A comparison of (1*a*) and (1*b*) in the $\theta = 0$ case clearly shows that the differences in the interference exponential terms have influenced the rate of convergence; hence in applications, the amplitude functions $A(x, y)$ in (7) may be significant in this respect. Differences in convergence of this type are often maintained in the rotated functions $(\theta = \pi/4)$.

To illustrate the comparison of the $\theta = 0$ and $\theta = \pi/4$ cases we use (1*a*), which is clearly converging well at CA(9, 9). A striking feature is that the errors are commonly out of phase in the half-ranges $0 \to \pm 1$; thus on a relative scale when the errors for $\theta = 0$ are small those for $\theta = \pi/4$ are large and vice versa. The errors in $x_s(y)$ on $[-1, 1]$ for the CA(7, 7) are shown in figure 1. We conjecture that the errors in both $x_s(y)$ and γ will be smaller, the nearer to one of the axes the singularities are. Thus in figure 2 the line of singularities is shown with respect to the $\theta = 0$ and $\theta = \pi/4$ axes. This rotation has moved one end of the interval $[1, -1]$ closer to an axis while the other end has been displaced further away.

Table 1. The errors in the estimates of the singularities $x_s(y)$ for functions (1*a*) and (1*b*) in units of 10^{-4} obtained from the diagonal CA sequences. The value of γ is $\frac{3}{2}$ and each function has been examined with ($\theta = \pi/4$) and without ($\theta = 0$) the rotation of the axes†.

	CA(3, 3)				CA(5, 5)				CA(7, 7)				CA(9, 9)			
y	(1*a*)		(1*b*)		(1*a*)		(1*b*)		(1*a*)		(1*b*)		(1*a*)		(1*b*)	
$\theta =$	0	$\pi/4$	0	$\pi/4$	0	$\pi/4$	0	$\pi/4$	0	$\pi/4$	0	$\pi/4$	0	$\pi/4$	0	$\pi/4$
−1·0	37	200	590	—	3	4	—	—	0·3	2	15	28	—	0·50	2·7	−17
−0·8	4	130	—	—	3	3	—	159	−1	1	9·6	14	0·08	0·30	5	−0·8
−0·6	−16	80	—	—	3	3	171	51	5	0·7	4·6	6	0·09	0·20	3	0·7
−0·4	−16	50	—	412	3	3	69	18	5	0·3	2·0	3	0·09	0·20	1	0·8
−0·2	4	20	202	165	3	3	22	9	−1	0·1	1·1	1·5	0·08	0·06	0·5	0·5
0	38	−3	141	95	3	3	—	7	0·3	−2	0·9	1·0	−0·20	0·08	0·3	1·5
0·2	83	−20	194	63	3	3	18	7	0·7	5	1·7	0·9	0·20	0·09	0·5	0·7
0·4	152	−20	139	43	3	3	48	6	2	4	8·0	0·7	0·30	0·09	12	0·5
0·6	311	−8	−97	24	4	3	141	5	3	—	51	0·5	0·90	0·08	130	0·4
0·8	864	11	−384	7	5	3	277	3	3	−0·1	162	0·2	2·0	0·08	374	0·3
1·0	—	40	−566	−5	7	3	335	2	4	0·1	262	0·2	2·0	0·05	517	—

Table 2. The errors in the estimates of the exponent γ corresponding to the CA in table 1, in units of 10^{-3}†

	CA(3, 3)				CA(5, 5)				CA(7, 7)				CA(9, 9)			
y	(1*a*)		(1*b*)		(1*a*)		(1*b*)		(1*a*)		(1*b*)		(1*a*)		(1*b*)	
$\theta =$	0	$\pi/4$	0	$\pi/4$	0	$\pi/4$	0	$\pi/4$	0	$\pi/4$	0	$\pi/4$	0	$\pi/4$	0	$\pi/4$
−1·0	20	160	700	—	10	10	—		3	11	150	238	—	4	43	−120
−0·8	−20	150	—	—	10	10	—	1000	−9	8	93	121	1	3	67	5
−0·6	−40	120	—	—	10	10	1000	277	−20	5	49	60	2	2	41	15
−0·4	−20	80	—	2000	10	10	330	110	−10	3	26	31	2	3	21	14
−0·2	20	40	800	1000	10	10	114	65	−5	2	16	19	1	1	9	10
0	80	−0·1	500	380	10	10	—	50	3	−30	13	13	−4	1	6	15
0·2	140	−30	600	236	10	10	78	41	10	−14	16	11	2	2	7	9
0·4	190	−30	430	154	10	10	140	33	10	−5	38	8	3	2	65	7
0·6	240	−30	−32	98	20	10	340	26	10		160	6	6	2	440	5
0·8	250	−0·2	−350	53	20	10	660	19	10	−1	440	3	10	1	1000	4
1·0	—	30	−440	15	20	10	900	13	10	3	−700	3	12	0	2000	—

† The dashes that appear in tables 1–5 correspond to no real roots in the approximants

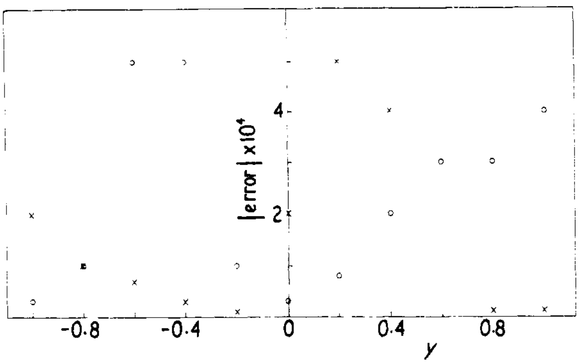

Figure 1. The errors in the CA(7, 7) to the singularities of function (1*a*) with ($\theta = \pi/4$, denoted by $\times$) and without ($\theta = 0$, denoted by $\bigcirc$) a rotation of the axes

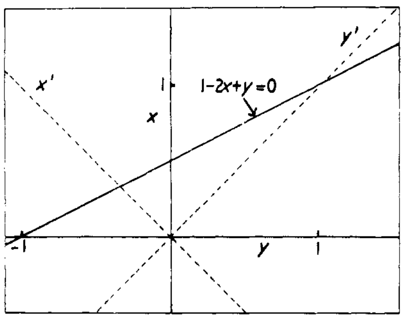

Figure 2. The locus of the singularities of function (1*a*) in relation to the original and rotated set of axes.

3. Functions with two sets of singularities: $(x-x_s(y))^{-\gamma}(x-x_{s'}(y))^{-\gamma'}$

The behaviour of the CA sequences for function (2*a*) is typical of the cases we have examined with two sets of singularities $x_s(y)$ and $x_{s'}(y)$; some of the results for the diagonal sequence CA(n, n) are shown in tables 3 and 4 where again we list the errors in the loci of the singularities, and the two exponents respectively. Convergence improves markedly beyond CA(5, 5), which is illustrated in figure 3, and an excellent fit to

$$x_s(y) \equiv 1-2x-\tfrac{1}{5}y = 0 \tag{9}$$

over $y = -0{\cdot}8$ to $0{\cdot}6$ is obtained at CA(9, 9), but a less accurate representation of the second line

$$x_{s'}(y) \equiv 1-x-\tfrac{1}{2}y = 0 \tag{10}$$

is reached by CA(9, 9). This difference in convergence between $x_s(y)$ and $x_{s'}(y)$ again reflects the fact that one can expect the results to be less accurate, the farther away the singularities are from the axes. The errors quoted for $x_{s'}(y)$ for $y < -0{\cdot}4$ may be related to the appearance of spurious roots; we have commonly observed that the approximants yield split real roots, or complex roots over subintervals of a locus $x_s(y)$.

A rotation of the axes can sometimes improve the approximants. This is illustrated in table 5, where the errors for the singularities and exponents of the function (2*b*) of

Table 3. Errors in the estimates of the singularities $x_s(y) \equiv 1-2x-\frac{1}{5}y = 0$, and $x_{s'}(y) \equiv 1-x-\frac{1}{2}y = 0$ in function (2*a*) obtained from the diagonal CA sequence. The errors are given in units of 10^{-4}. The points marked * correspond to the probably spurious points shown in figure 3.

	CA(5, 5)		CA(7, 7)		CA(9, 9)	
y	$x_s(y)$	$x_{s'}(y)$	$x_s(y)$	$x_{s'}(y)$	$x_s(y)$	$x_{s'}(y)$
−1·0	−90	−7000*	−110	−8000*	—	—
−0·8	−70	−5000*	−70	−7000*	7	—
−0·6	−40	−2000*	−30	−7000*	−2	−150
−0·4	−20	−600	−5	−550	−1·5	40
−0·2	−6	−90	8	−200	−1·1	10
0	−3	−47	−6	−70	−0·6	−2
0·2	−1·2	−15	−2	−20	−0·2	−2
0·4	−1.1	50	−0·1	−9	−0·03	−0·2
0·6	0·7	150	0·3	−20	+0·04	6
0·8	−30	320	13	−60	—	24
1·0	−100	570	60	−170	—	97

Table 4. Errors in the residues $\gamma = \frac{1}{2}$ and $\gamma' = \frac{3}{2}$ of the singularities $x_s(y)$ and $x_{s'}(y)$ in table 4, in units of 10^{-3}. The points marked * correspond to the probably spurious points shown in figure 3.

	CA(5, 5)		CA(7, 7)		CA(9, 9)	
y	γ	γ'	γ	γ'	γ	γ'
−1·0	−250	−1500*	−260	−1400*	—	—
−0.8	−180	−1200*	−190	−1300*	−50	—
−0.6	−110	−400*	−110	−1500*	−52	160
−0·4	−63	−50	−44	−200	−23	−106
−0·2	−33	13	73	−42	−20	14
0	−17	−0·2	−8	−8	−10	8
0·2	−8	3	−8	−0·1	−5	4
0·4	−3	37	−4	−0·4	−2	2
0·6	−0·1	110	−2	−12	1	0·2
0·8	11	200	−8	−34	—	−13
1·0	70	300	−87	2	—	−160

CA(9, 9) are given. Even though the results for $x_s(y)$ are very good over the whole range, the errors in the region $y \to 1$ can be reduced considerably by rotating the axes; the errors in brackets are those obtained using a rotation of $\theta = \pi/4$. This operation is illustrated in figure 4, where the area of improvement is the region marked R; thus only one interval of the y range near $y = 1$ will be improved on the line

$$x_{s'}(y) \equiv 1-\tfrac{1}{2}x-\tfrac{1}{2}y = 0 \tag{11}$$

since this line is parallel to and far away from the new x axis. This is reflected in table 5, where real roots are obtained only for the last two values of y.

Our overall conclusions from numerical experiments of this type using the diagonal and symmetric off-diagonal approximants are that the CA$(n, n+j)$ $(j = 0, \pm 1)$ sequences compare favourably with results obtainable using Padé approximants on single-variable

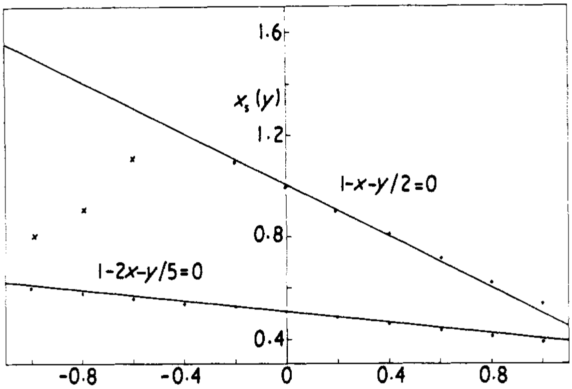

Figure 3. The estimates of $x_s(y)$ and $x_{s'}(y)$ (equations (9) and (10)) obtained from the CA(5, 5) to function (2*a*). × denotes probably spurious roots.

Table 5. The errors in the singularities $x_s(y) \equiv 1-x-\frac{1}{2}y=0$ and $x_{s'}(y) \equiv 1-\frac{1}{2}x-\frac{1}{2}y=0$ in units of 10^{-4}, and the errors in the exponents $\gamma=\frac{3}{2}$ and $\gamma'=\frac{5}{4}$ in units of 10^{-3} of the function (2*b*) obtained from the CA(9, 9). The figures in brackets are the corresponding errors obtained under a rotation of the axes through $\pi/4$, where an approximation to the real root is obtained.

y	$x_s(y)$	γ	$x_{s'}(y)$	γ'
−1·0	1 (1)	12 (10)	—	—
−0·8	1 (1)	8 (8)	—	—
−0.6	0·7 (1)	5 (9)	−60	−430
−0·4	0·3 (4)	2 (20)	−300	−150
−0·2	0·1 (7)	1 (20)	−110	−56
0	0·07 (7)	0·6 (20)	−30	−20
0·2	0·02 (3)	0·3 (10)	−11	−59
0·4	1 (0·08)	1 (3)	−60	15
0·6	1 (0·06)	4 (0·3)	−80	2
0·8	3 (−0·004)	10 (0·01)	−150 (20)	80 (40)
1·0	7 (−0·04)	28 (0·3)	— (−1)	— (−0·4)

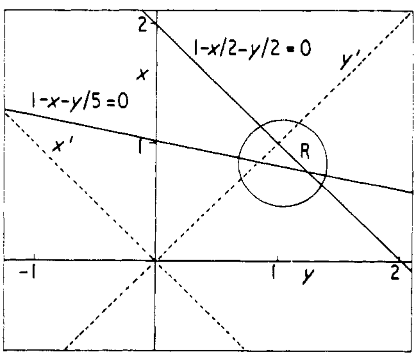

Figure 4. R is the region of improvement in the estimates of $x_s(y)$ and $x_{s'}(y)$ shown in table 5 on using the rotation operation.

power series (Hunter and Baker 1973) when the singularities lie close to one of the axes. This effect is seen clearly in II in determining the variations of the critical temperature $T_c(\alpha)$ with variations in some microscopic parameter α, using series expansions known in the field of critical phenomena. Although these approximants are not covariant under rotations of the axes, we have demonstrated that it can be a useful procedure to perform this operation, which is likely to be a necessary operation in many applications.

Acknowledgments

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References

Baker G A and Gammel J L 1970 *The Pade Approximant in Theoretical Physics* (New York: Academic Press)
Chisholm J S R 1973 *Math. Comput.* **27** 841–8
Chisholm J S R and McEwan J 1974 *Proc. R. Soc.* A **336** 421–52
Gaunt D S and Guttmann A J 1974 *Phase Transitions and Critical Phenomena*, vol 3 eds C Domb and M S Green (New York: Academic Press) pp 181–242
Graves-Morris P, Hughes-Jones R and Makinson 1974 *J. Inst. Math. Applic.* **13** 311–20
Graves-Morris P and Roberts D 1975a *Commun. Comput. Phys.* **9** 46–50
—— 1975b *University of Kent, Canterbury Preprint* UKC, AM/PRGM and DER
Graves-Morris P and Samwell C J 1975 *J. Phys.* G: *Nucl. Phys.* in the press
Hughes-Jones R 1973 *University of Kent, Canterbury Preprint* UKC, AM/RHJ/3
Hughes-Jones R and Chisholm J S R 1975 *Proc. R. Soc.* to be published
Hughes-Jones R and Graves-Morris P 1974 *Brookhaven Preprint* AMD 674
Hunter D L and Baker G A 1973 *Phys. Rev.* **137** 3346–92
Lutterodt 1974 *J. Phys.* A: *Math., Nucl. Gen.* **7** 1027–37
Watson P J S 1974 *J. Phys.* A: *Math., Nucl. Gen.* **7** L167–70
Wood D W and Fox P F 1975 *J. Phys.* A: *Math. Gen.* **8** in the press
Wood D W and Griffiths H P 1974 *J. Phys.* A: *Math., Nucl Gen.* **7** L101–4