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1974 J. Phys. A: Math. Nucl. Gen. 7 L101

(http://iopscience.iop.org/0301-0015/7/9/001)

J. Phys. A: Math., Nucl. Gen., Vol. 7, No. 9, 1974. Printed in Great Britain. © 1974

LETTER TO THE EDITOR

Chisholm approximants and critical phenomena

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Received 11 April 1974

Abstract. Recent developments in rational approximation schemes defined from power series of many variables are discussed in relation to their application to problems in critical phenomena. A detailed calculation is performed on an Ising model problem which illustrates the use of these new approximants in the two-variable case.

During the last decade the Padé approximant scheme of rational approximation defined from several terms of a power series

$$f(z) = \sum_n c_n z^n \tag{1}$$

has proved an effective way of approximating $f(z)$ in many branches of theoretical physics. (For a review see Baker and Gammel 1970.) Perhaps the most spectacular success of Padé approximants has been in the field of critical phenomena, where they have been extensively employed to determine the nature of the thermodynamic functions in their approach to the critical point singularity. (For reviews see Fisher 1967, Gaunt and Guttmann 1972 and Hunter and Baker 1973.)

Recently Chisholm (1973) has proposed a scheme of rational approximants defined from a double power series

$$g(z_1, z_2) = \sum_n \sum_m c_{n,m} z_1^n z_2^m \tag{2}$$

and Chisholm and McEwan (1974) have now extended Chisholm's original two-variable approximants into a rational approximation scheme defined from a power series in N variables. These N-variable approximants possess many of the algebraic properties of Padé approximants (for details see Chisholm and McEwan 1974) and in addition possess the projective property that if any k variables are equated to zero, the approximants in $N-k$ variables formed from the corresponding power series are obtained. Thus in the two-variable case, the diagonal approximants $CA(m, m)$ to (2), which are defined in the form

$$CA(m, m) = \frac{\sum_i^m \sum_j^m a_{ij} z_1^i z_2^j}{\sum_k^m \sum_l^m b_{kl} z_1^k z_2^l} \tag{3}$$

reduce to the $[m, m]$ Padé approximants for $g(0, z_2)$, and $g(z_1, 0)$ when $z_1 = 0$ and $z_2 = 0$ respectively.

This new approximation method is well suited to the analysis of many problems that arise in critical phenomena, where the expansions of the thermodynamic functions are developed naturally in terms of two or more variables. (For examples of such expansions see Sykes *et al* 1973, Wood and Griffiths 1973, 1974, and Wood and Dalton 1972.)

We consider two illustrative examples of the use of Chisholm approximants (CA) in critical phenomena, and compare their performance with Padé approximants. From a viewpoint of physical interest, the first case we have chosen is a simple one where the two variables relate to the two coupling constants J_1, and J_2 in a three-dimensional Ising model with nearest neighbour (NN), and next nearest neighbour (NNN) pair interactions (Dalton and Wood 1969).

The high temperature expansion of the zero-field susceptibility χ_0 can be put in the form of a double power series

$$\chi_0 = 1 + \sum_l P_l(\alpha)K^l, \tag{4}$$

where $\alpha = J_2/J_1$, $K = J_1/kT$, and $P_l(\alpha)$ is a polynomial of degree l in α. We take the BCC lattice as an example for which the polynomial coefficients are known up to $P_6(\alpha)$ (Dalton and Wood 1969).

The behaviour of the susceptibility in the neighbourhood of the critical singularity is taken to have the asymptotic form

$$\lim_{K\to K_c(\alpha)} \chi_0(K,\alpha) \sim A(K,\alpha)(K_c(\alpha) - K)^{-\gamma}. \tag{5}$$

We have calculated examples of the $CA(m, n)$ to the expansion of

$$\frac{\partial}{\partial K}[\ln \chi_0(K,\alpha)] \sim \left.\frac{\gamma}{K_c(\alpha) - K}\right|_{K\to K_c(\alpha)} \tag{6}$$

which are approximants yielding unbiased estimates of the *functions* $K_c(\alpha)$, and $\gamma(\alpha)$ (Hunter and Baker 1973). To ensure the existence of the Chisholm approximants for expansions of the type (4) we initially effect the transformation

$$\begin{aligned} K &= x + y \\ \alpha &= x - y \end{aligned} \tag{7}$$

on the series expansion (preserving the origin), and subsequently perform the inverse transformation on the calculated $CA(m, n)$, which have the final form

$$CA(m,n) = \frac{\Sigma_i^{2m}\Sigma_j^{2m} a_{ij}\alpha^i K^j}{\Sigma_k^{2n}\Sigma_l^{2n} b_{kl}\alpha^k K^l}. \tag{8}$$

Clearly the approximants (8) effect an approximation to the line of singularities $T_c = T_c(\alpha)$ through the solution of

$$\sum_k^{2n}\sum_l^{2n} b_{kl}\alpha^k K^l = 0. \tag{9}$$

The usefulness of the Chisholm approximants is now evident here, each member of the sequence $CA(m, n)$ is approximating the functional relation determining the line of singularities $K_c(\alpha)$, to obtain the corresponding information from Padé approximants the initial series must be sampled at various selected values of α, and the calculations repeated at each sampling point. How well and over what range the Chisholm approximants will generally approximate the line of singularities is presently being investigated by the authors, but the projective property of the CA for the present example would perhaps suggest that a good fit could be expected for small values of α. Over such a range we would also obtain estimates of the critical exponent *function* $\gamma(\alpha)$, thus we have the prospect of obtaining a direct functional representation of the behaviour of the critical exponents generally when additional perturbing interactions are added to a basic interaction hamiltonian.

We have obtained the $CA(2, 2)$ to (6) and compared the results for $K_c(\alpha)$ with those of Dalton and Wood (1969), which are probably accurate to within 5 parts in 10^4, and based upon a biased Padé approximant analysis. The results are displayed in table 1. The $CA(2, 2)$ begins to depart from a good approximation to $K_c(\alpha)$ at about $\alpha = 0{\cdot}4$, and initially performs very well in the range 0–0·3 giving an extremely good unbiased fit to the changing critical point. The results for the critical exponent γ (which is thought to be $\frac{5}{4}$, and independent of α) are very revealing. Firstly the approximation to 1·25 is very good, but more significantly the index is clearly seen to be invariant to α over the range for which a good fit is obtained to the singularity. Following recent developments in the universality postulate (Griffiths 1970, Kadanoff 1973, Wilson 1971), there remains little debate about the invariance of γ in this instance, and the Chisholm approximant is yielding a direct numerical prediction of this invariance.

Table 1. The location of the critical point singularity $K_c(\alpha)$, and the critical exponent $\gamma(\alpha)$ obtained from the $CA(2, 2)$ to (6).

α	$K_c(\alpha)$ from the $CA(2, 2)$	$K_c(\alpha)$ from Dalton and Wood (1969)	$\gamma(\alpha)$ from the $CA(2, 2)$
0	0·1577	0·1573	1·261
0·1	0·1453	0·1450	1·263
0·2	0·1351	0·1344	1·263
0·3	0·1277	0·1253	1·267
0·4	0·1243	0·1175	1·281

The second example is taken from Griffiths and Wood (1973), where the low temperature ($T < T_c$) expansion of the zero-field magnetization function M_0 for an Ising model triangular lattice (two-dimensional) which includes both two-body and three-body coupling constants (J_2, and J_3) can be put in the form

$$M_0 = 1 + \sum_n \sum_m c_{n,m} u_2^n u_3^m \tag{10}$$

where $u_{2,3} = \exp(-4J_{2,3}/kT)$, the coefficients $c_{n,m}$ are given by Griffiths and Wood (1973), and we use α to denote J_3/J_2.

The behaviour of the magnetization in the neighbourhood of the critical point $u_{2,c}(\alpha)$ is assumed to have the form

$$\lim_{u_2 \to u_{2,c}(\alpha)} M_0(u_2, u_3) \sim B(u_2, u_3)(u_2 - u_{2,c}(\alpha))^{\beta(\alpha)} \tag{11}$$

where the line of critical points is traced out by the function $u_{2,c}(\alpha)$. To form approximations to the functions $u_{2,c}(\alpha)$ and $\beta(\alpha)$ we can form the $CA(m, n)$ to the two partial derivatives

$$\frac{\partial}{\partial u_2}[\ln M_0(u_2, u_3)] \sim \frac{r_1(\alpha)}{u_2 - u_{2,c}(\alpha)} \tag{12}$$

and

$$\frac{\partial}{\partial u_3}[\ln M_0(u_2, u_3)] \sim \frac{r_2(\alpha)}{u_2 - u_{2,c}(\alpha)} \qquad (13)$$

where transformations similar to (7) must again be included.

For these expansions the two-residue functions $r_1(\alpha)$ and $r_2(\alpha)$ in (12) and (13) are related to the exponent $\beta(\alpha)$ by

$$\beta(\alpha) = r_1 + \alpha u_{2,c}(\alpha)^{\alpha-1} r_2 . \qquad (14)$$

We include here just a single comparison of two low-order approximants, these are (i) the [6, 6] Padé approximant to (12) with $u_2 = u_3$, and (ii) the $CA(4, 4)$ to (12) and (13) each examined at the point $\alpha = 1$. The estimates from (i) are $u_{2,c}(1) = 0{\cdot}4976$, and $\beta(1) = 0{\cdot}074$, while the approximants in (ii) yield $u_{2,c}(1) = 0{\cdot}4911$ from (12), $u_{2,c}(1) = 0{\cdot}4962$ from (13) and $\beta(1) = 0{\cdot}063$ from (14). Only a relatively small number of terms in the series are being used in each of these approximant schemes in the above case, consequently the estimates themselves are probably some way off convergence, however we see that the two schemes are yielding similar results in the region $\alpha \to 1$.

Recently Wood and Griffiths (1974) have reported evidence that the critical exponent β may depend upon the relative admixtures of many-body potential terms in the interaction hamiltonian for models of the above type. The Chisholm approximants provide the ideal approximation scheme for investigating any variations in critical exponents, and are currently being studied in this context by the authors, they are also being applied to a wide variety of series expansions in lattice statistics.

It is a pleasure to acknowledge the generous encouragement of Professor Chisholm, and the expert assistance of Dr David Roberts in the establishment of the CA computer program on the Nottingham University 1906A computer.

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