On the recurrence relation method of series analysis

1975 J. Phys. A: Math. Gen. 8 1081

(http://iopscience.iop.org/0305-4470/8/7/011)

J. Phys. A: Math. Gen., Vol. 8, No. 7, 1975. Printed in Great Britain.

On the recurrence relation method of series analysis

A J Guttmann

Department of Mathematics, University of Newcastle, New South Wales 2308, Australia

Received 24 February 1975, in final form 14 March 1975

Abstract. The recurrence relation method of series analysis is tested on the 12 test functions recently used by Baker and Hunter to study various methods of series analysis. It is found that the recurrence relation method is demonstrably superior to other methods for about half the test functions, and that for no test function is it significantly worse than existing methods.

1. Introduction

In two recent articles Baker and Hunter (1973) critically reviewed most of the existing methods for the analysis of power series expansions that arise in theoretical physics. The principal thrust of their work was to study those methods particularly suited to the analysis of series which arise in lattice statistical problems. Following a critical review they developed a number of generalizations and extensions of existing methods.

In order to compare various methods they used a number of example series that include, in various combinations, most of the types of singular behaviour generally conjectured for the lattice statistical thermodynamic functions. The test functions given by Hunter and Baker (1973) are reproduced in table 1. These functions were expanded to 10, 15 and 20 terms and then analysed in order to determine the principal critical exponent $\gamma = 1{\cdot}5$ and corresponding critical point $x_c = 1$. The accuracy of the estimates was stated by evaluating the quantity $\epsilon_n = -\lg \rho_n$ where ρ_n is the relative error in estimating one of the critical parameters from n terms in the series expansion.

Table 1. Test functions A–L used to study the various methods of series analysis (from Hunter and Baker 1973).

Function A	$(1-x)^{-1\cdot5}+\mathrm{e}^{-x}$
Function B	$(1-x)^{-1\cdot5}(1+\frac{1}{2}x)^{1\cdot5}+\mathrm{e}^{-x}$
Function C	$(1-x)^{-1\cdot5}(1-\frac{1}{2}x)^{1\cdot5}+\mathrm{e}^{-x}$
Function D	$(1-x)^{-1\cdot5}+(1+\frac{1}{4}x^2)^{-1\cdot25}+(1+\frac{15}{112}x-\frac{1}{4}x^2)^{-1\cdot25}$
Function E	$(1-x)^{-1\cdot5}(1+\frac{1}{2}x)^{1\cdot5}+(1+\frac{1}{4}x^2)^{-1\cdot25}+(1+\frac{15}{112}x-\frac{1}{4}x^2)^{-1\cdot25}$
Function F	$(1-x)^{-1\cdot5}(1-\frac{1}{2}x)^{1\cdot5}+(1+\frac{1}{4}x^2)^{-1\cdot25}+(1+\frac{15}{112}x-\frac{1}{4}x^2)^{-1\cdot25}$
Function G	$(1-x)^{-1\cdot5}+\{2(1-x)(2-x)^6/[(2-x)^7-x^7]\}^{1\cdot25}$
Function H	$(1-x)^{-1\cdot5}(1+\frac{1}{2}x)^{1\cdot5}+\{2(1-x)(2-x)^6/[(2-x)^7-x^7]\}^{1\cdot25}$
Function I	$(1-x)^{-1\cdot5}(1-\frac{1}{2}x)^{1\cdot5}+\{2(1-x)(2-x)^6/[(2-x)^7-x^7]\}^{1\cdot25}$
Function J	$(1-x)^{-1\cdot5}+(1+\frac{4}{5}x)^{-1\cdot25}$
Function K	$(1-x)^{-1\cdot5}+(1+\frac{4}{5}x)^{-1\cdot25}+\mathrm{e}^{-x}$
Function L	$-(1-x)^{-1\cdot5}\ln(1-x)$

The purpose of the present paper is to apply a new method of series analysis, called the recurrence relation method (Guttmann and Joyce 1972, Joyce and Guttmann 1973), to the example series given by Baker and Hunter, and thereby to compare this method with the existing methods.

In general the new method is found to compare favourably with existing methods. For about half the test functions it gives better results than any existing method, while for no function are the results significantly worse than for existing methods.

For a general guide to methods of series analysis other than the recurrence relation method, and an introduction to the whole problem of series analysis, reference should be made to Gaunt and Guttmann (1974).

2. The recurrence relation method

This method is described by Guttmann and Joyce (1972) and Joyce and Guttmann (1973). Briefly, in its simplest form, it involves fitting the available series coefficients $c_0, c_1, c_2, \ldots, c_n$ to a recurrence relation of the form

$$R_{2,M}(c_n) = \sum_{i=0}^{M} [A_{i,2}(n-i)^2 + A_{i,1}(n-i) + A_{i,0}]c_{n-i} = 0 \qquad (2.1)$$

where $A_{0,2} \equiv 1, A_{0,0} \equiv 0$ and $c_{-n} = 0\,(n > 0)$. The coefficients

$$\{A_{0,1}; A_{i,2}, A_{i,1}, A_{i,0}; i = 1, 2, \ldots, M\}$$

are determined quite readily from the series coefficients by solving a system of linear equations. This recurrence relation can then be solved by noting that if the coefficients c_n satisfy (2.1), then the function defined by

$$f(z) = \sum_{n=0}^{\infty} c_n z^n \qquad (2.2)$$

satisfies a second-order linear differential equation whose critical properties can be obtained by standard techniques (Ince 1927). Further details of the method are given in the references cited above. It should be pointed out, however, that the method is a natural generalization of the Padé approximant method applied to the logarithmic derivative of a series, since in that case the Padé method can be shown to be expressible as a first-order linear differential equation. The method receives its inspiration from the fact that the Onsager (1944) solution for the zero-field internal energy satisfies a recurrence relation of the precisely assumed form, as shown by Joyce (unpublished).

Without further ado we will demonstrate the application of this method to the 12 test functions given in table 1.

3. Numerical experiments

For all 12 functions the principal critical point $x_c = 1$, and the corresponding exponent $\gamma = 1{\cdot}5$. The three standard methods used by Hunter and Baker (1973) were the ratio method (R), which was then refined by the use of Neville tables (N), and the Padé approximant method (P). Further, three new methods were given by Baker and Hunter (1973): the generalized Padé approximant method (GPA), the exponent renormalization method

(ER) and the confluent singularity method (CS). All these methods were applied to the given series by Baker and Hunter and the results which we quote for these methods are theirs. The results are compared with our recurrence relation (RR) method in the remainder of this section.

In table 2 we compare estimates of the critical point x_c by quoting $\epsilon_n = -\lg \rho_n$ where ρ_n is the relative error in x_c using n series coefficients. Note that while the results of Baker and Hunter are quoted for 10, 15 and 20 terms, the nature of the RR method is

Table 2. Summary of analysis of the 12 test series for estimates of the critical point $x_c = 1{\cdot}0$. The numbers quoted are the values of the parameter $\epsilon = -\lg(\Delta x_c/x_c)$.

Test series	Number of terms used	R	N	P	GPA [1, D, M]	$\gamma = 1{\cdot}5$ ER	RR	Number of terms used in RR
	10	3·2		2·7		7·0	>13	10
A	15	8·1		4·0		>7·0	>13	13
	20	13·9		4·8	>10	>7·0	>13	19
	10	2·3	2·4	2·7		2·5	>13	10
B	15	2·8	3·8	3·9		3·5	>13	13
	20	3·1	5·4	5·1	3·5	4·0	>13	19
	10	2·3		2·5		2·3	3·2	10
C	15	2·5	4·1	3·4		3·1	4·1	13
	20	2·9	5·7	4·0	3·1	3·7	>13	19
	10	1·7		1·9		3·1	—	10
D	15	2·6		2·2		4·7	2·0	13
	20	3·6		3·5	5·4	7·0	4·0	19
	10	1·6		1·3		1·9	—	10
E	15	2·4		2·5		3·2	2·0	13
	20	3·0	3·9	3·7	3·8	4·0	3·6	19
	10	1·5		1·1		1·9	0·9	10
F	15	2·8		1·4		2·7	1·7	13
	20	3·0		2·7	2·9	3·1	5·4	19
	10	1·4		1·3		2·4	3·2	10
G	15	1·6		1·3		3·3	2·1	13
	20	1·9		2·7	2·3	4·5	2·0	19
	10	1·6		1·7		2·2	2·7	10
H	15	2·0		1·8		2·7	2·8	13
	20	2·2		2·4	2·5	3·2	2·0	19
	10	1·0		0·9		2·0	2·0	10
I	15	1·2		1·4		2·2	1·7	13
	20	1·5		2·2	1·6	2·4	2·6	22
	10	1·1	1·5	2·2		6·7	>13	10
J	15	1·7	2·2	3·5		>7·0	>13	13
	20	2·0	2·8	4·4	7·2	>7·0	>13	19
	10	1·1		0·7		5·2	2·4	10
K	15	1·7	2·2	3·0		>7·0	3·2	13
	20	2·0	2·6	3·9	6·5	>7·0	5·3	19
	10	1·6	2·9	2·7	not	not	>13	10
L	15	1·9	3·3	3·2	given	given	>13	13
	20	2·2	3·5	3·6			>13	19

such that the number of coefficients at each step increases by three; hence our results are for 10, 13 and 19 terms, except for the isolated case of series *I*, where due to a numerical difficulty we have given the result ϵ_{22} instead of ϵ_{19}. A dash in the RR column indicates that no singularity on the positive real axis is predicted in that approximation. Our computer program prints out estimates to only 13 significant digits, hence the maximum value of ϵ_n that can be obtained is 13.

From table 2 we see that with only 10 coefficients, functions *A*, *B*, *J*, *L* have their critical points determined to machine accuracy. In fact it can be shown (Joyce and Guttmann 1973) that these functions can be determined precisely by the RR method, given 10 series coefficients. For the other series the RR method is clearly more accurate than any other for function *C*. For functions *F*, *H*, *I* it is of comparable accuracy to the ER method. The ER method could, however, be called a 'quasi-biased' method since it includes the exponent estimate $\gamma = 1{\cdot}5$. Leaving aside the ER results we find that the RR method is now the most accurate method for functions *F* and *I* as well, and is of comparable accuracy to the R, N and P methods for functions *D*, *E*, *G*, *H*, *K*, but in each case ϵ_{19} is slightly worse than ϵ_{20} for the [1, *D*, *M*] GPA.

Turning now to table 3 we give the ϵ_n values for estimates of the critical exponent γ. Exactly the same conclusions apply as for ϵ_n values of x_c in table 2. The asterisks for example *L* imply that the output indicates the presence of a confluent logarithmic

Table 3. Summary of analysis of the 12 test series for estimates of the critical exponent $\gamma = 1{\cdot}5$. The numbers quoted are the values of the parameter $\epsilon = -\lg(\Delta\gamma/\gamma)$.

Test series	Number of terms used	R	N	P	GPA [1, *D*, *M*]	RR	Number of terms used in RR
	10	2·4		1·7		>13	10
A	15	7·1		2·6		>13	13
	20	12·8		3·0	>10	>13	19
	10	1·3		1·7		>13	10
B	15	1·6	2·3	2·5		>13	13
	20	1·7	3·4	3·3	1·9	>13	19
	10	1·0		1·2		1·9	10
C	15	1·3	2·7	2·2		3·3	13
	20	1·4	3·7	2·4	1·5	>13	19
	10	0·8		0·7		—	10
D	15	1·4		1·0		0·8	13
	20	2·0		1·9	4·3	2·4	19
	10	0·7		0·4		—	10
E	15	1·3		1·4		0·7	13
	20	1·7		2·2	1·7	2·1	19
	10	0·8		0·3		−0·4	10
F	15	1·1		0·3		0·5	13
	20	1·5		1·2	1·5	2·8	19
	10	0·6		0·4		1·7	10
G	15	0·6		0·4		1·2	13
	20	0·9		1·3	1·2	0·7	19
	10	0·7		0·7		2·5	10
H	15	0·9		0·9		1·7	13
	20	1·3		1·3	1·7	1·2	19

Table 3—continued

Test series	Number of terms used	R	N	P	GPA $[1, D, M]$	RR	Number of terms used in RR
	10	0·1		−0·4		0·9	10
I	15	0·1		2·3		0·8	13
	20	0·4		1·3	0·4	1·5	19
	10	0·2		1·4		>13	10
J	15	0·5		2·2		>13	13
	20	0·8		2·7	6·3	>13	19
	10	0·1		0·1		1·2	10
K	15	0·5		1·7		1·9	13
	20	0·8		2·3	5·5	3·4	19
	10	0·3		0·7	not	<13*	10
L	15	0·4	0·8	0·8	given	>13*	13
	20	0·5	0·9	0·8		>13*	19

singularity whose precise nature is revealed by further analysis (Joyce and Guttmann 1973). To illustrate this, the output for the case $n = 13$, corresponding to $\text{R}_{2,4}$, is given in table 4. The fact that the real root is printed out as a double root indicates a confluent

Table 4. The output from the recurrence relation program for test series *L* assuming that 13 series coefficients are known. The double real root at $x = 1$ indicates a confluent logarithmic singularity (see text).

Real root	Imaginary root	Real exponent	Imaginary exponent
1·000000000000	−0·0000000143439	−283·28308081	
1·000000000000	−0·0000000143439	−283·28308081	
−0·341142903637	−2·5947355044	0·999999999971	0·000000000012856
−0·341142903637	2·5947355044	1·000000000001	−0·000000000024339

logarithmic singularity. An identical situation exists in the Onsager solution for the internal energy of the square lattice Ising model. In this situation the exponent printed out is spurious and is a measure only of the working precision of the arithmetic unit on the computer. Further analysis (Joyce and Guttmann 1973) assuming a confluent singularity is needed to identify the correct exponent. The other two singularities are also spurious and are analogous to the branch cuts placed down by the Padé method.

In table 5 we list the ϵ_n values for biased estimates of the exponent γ. These estimates are biased in that we have fed in the position of the critical point. It is no more difficult to do this in the RR method than in the Padé method. As can be seen from the table, the RR method is demonstrably superior for functions *A*, *B*, *C*, *F*, *H*, *I*, *J*, *K*, *L* and of comparable accuracy to existing methods for the remaining functions *D*, *E*, *G*.

Finally, in table 6 we list the ϵ_n values for all the identifiable critical points, not just the physical singularity. Again the RR method is superior for functions *A*, *B*, *C*, *F*, *I*, *J*, *K*. For functions *D*, *E* the RR method is about as good as the GPA or P method, while for functions *G*, *H* the standard Padé method has the edge over both our method and the GPA method.

Table 5. Summary of analysis of the 12 test series for biased estimates of the critical exponent $\gamma = 1{\cdot}5$, given the critical point $x_c = 1$. The numbers quoted are the values of the parameter $\epsilon = -\lg(\Delta\gamma/\gamma)$.

Test series	Number of terms used	R	N	P	RR	Number of terms used in RR
	10	4·1		2·4	>13	10
A	15	9·4		3·0	>13	13
	20	15·4		3·6	>13	19
	10	1·7	2·5	2·7	>13	10
B	15	1·9	3·8	3·3	>13	13
	20	2·0	5·8	3·7	>13	19
	10	1·3	1·8	1·7	2·0	10
C	15	1·5	3·6	2·4	3·4	13
	20	1·6	5·4	3·1	>13	19
	10	1·5		1·0	1·7	10
D	15	2·6		1·9	1·5	13
	20	3·7		2·3	3·5	19
	10	1·6		1·3	1·5	10
E	15	1·8		1·8	1·0	13
	20	2·0	2·8	2·4	3·5	19
	10	0·8		0·4	1·5	10
F	15	1·3		1·2	2·0	13
	20	1·6	1·8	1·8	3·5	19
	10	1·3		0·8	1·6	10
G	15	1·4		1·1	0·9	13
	20	1·5		2·0	1·5	19
	10	1·5		0·5	1·8	10
H	15	1·6		1·2	1·7	13
	20	1·6		1·7	2·0	19
	10	0·8		0·6	1·1	10
I	15	0·8		0·8	0·9	13
	20	1·2		1·7	2·0	19
	10	0·7		1·7	>13	10
J	15	1·2		2·7	>13	13
	20	1·4		3·2	>13	19
	10	0·7		1·4	2·8	10
K	15	1·2		2·0	3·1	13
	20	1·4		2·5	5·3	19
	10	0·5	0·8	0·8	>13	10
L	15	0·6	0·9	0·9	>13	13
	20	0·7	0·9	0·9	>13	19

4. Conclusion

As can be seen from the numerical evidence, the RR method constitutes a valuable tool in the analysis of series expansions. Its worth in a practical example has already been demonstrated by Wheeler *et al* (1974) who use the method to analyse spectral densities using modified moments. The method is currently being applied to a number of Ising

Table 6. Comparison of accuracy of estimates (assuming 19 or 20 terms) of the locations of the singularities in functions *A–K*. The numbers quoted are the values of the parameter $\epsilon = -\lg(|\Delta x_c^i|/|x_c^i|)$, where x_c^i refers to the *i*th singularity of the test function.

Test series	i	Exact location of singularity x_c^i	ϵ_{20} for generalized approximant analysis	ϵ_{20} for usual Padé approximant analysis	ϵ_{19} for RR analysis
A	1	1·0000	>10	4·8	>13
B	1	1·0000	3·5	5·1	>13
C	1	1·0000	3·1	4·0	>13
D	1	1·0000	5·4	3·5	4·0
	2	−1·7500	1·7	2·2	4·7
	3, 4	±2·0000i	1·7	2·0	2·0
	5	2·2857	1·1	—	—
E	1	1·0000	3·8	3·7	3·6
	2	−1·7500	1·4	2·2	1·9
	3, 4	±2·0000i	0·7	1·8	1·2
	5	2·2857	—	—	−0·1
F	1	1·0000	2·9	2·7	5·4
	2	−1·7500	1·6	2·1	3·0
	3, 4	±2·0000i	1·5	2·0	2·0
	5	2·2857	—	—	—
G	1	1·0000	2·3	2·7	2·0
	2, 3	1·0000±0·4816i	0·5	0·9	0·6
	4, 5	1·0000±1·2540i	—	0·5	0·9
	6, 7	1·0000±4·3813i	—	0·5	—
H	1	1·0000	2·5	2·4	2·0
	2, 3	1·0000±0·4816i	0·6	0·9	−0·2
	4, 5	1·0000±1·2540i	—	0·5	0·6
	6, 7	1·0000±4·3813i	—	0·2	—
I	1	1·0000	1·6	2·2	2·6
	2, 3	1·0000±0·4816i	—	1·0	1·2
	4, 5	1·0000±1·2540i	—	1·0	1·4
	6, 7	1·0000±4·3813i	—	0·7	0·7
J	1	1·0000	7·2	4·4	>13
	2	−1·2500	2·0	4·2	>13
K	1	1·0000	6·5	3·9	5·3
	2	−1·2500	2·1	2·7	5·1

model and spherical model series by Guttmann, Joyce and Rehr and it is hoped to publish these results shortly. A fuller discussion of the method and its generalizations will be published shortly. Generalizations that have proved valuable include extensions to higher-order recurrence relations, specification of critical points and critical exponents of one or more singularities, specifications of the positions of double roots and their exponents, and variations in the nature of the analytic structure of the differential equation corresponding to the recurrence relation, both at the origin and at infinity.

It should be noted that for the standard methods of analysis, such as the R and P methods, there do exist results on convergence that are sometimes applicable. At the present state of development, no such results are known for the RR method.

Note also that the RR method gives an exact representation for a wider class of functions than do the other methods tested, but there are several functions here which cannot be represented exactly by recurrence relations—at least not without a prohibitively large number of terms in the recurrence relation.

Acknowledgments

The recurrence relation method described here was devised together with Dr G S Joyce and followed a suggestion by Dr M F Sykes. Improvements to the computer program were made by Dr J J Rehr. The author wishes to express his indebtedness to all these people, and thanks the referee for useful comments.

This work was supported (in part) by the Australian Research Grants Committee.

References

Baker G A Jr and Hunter D L 1973 *Phys. Rev.* B **7** 3377–92

Gaunt D S and Guttmann A J 1974 *Phase Transitions and Critical Phenomena* vol 3, eds C Domb and M S Green (London and New York: Academic Press) pp 181–244

Guttmann A J and Joyce G S 1972 *J. Phys.* A: *Gen. Phys.* **5** L81–4

Hunter D L and Baker G A Jr 1973 *Phys. Rev.* B **7** 3346–76

Ince E L 1927 *Ordinary Differential Equations* (London: Longmans)

Joyce G S and Guttmann A J 1973 *Padé Approximants and their Applications* ed P R Graves-Morris (London and New York: Academic Press) pp 163–7

Onsager L 1944 *Phys. Rev.* **65** 117–49

Wheeler J C, Prais M G and Blumstein C 1974 *Phys. Rev.* B **10** 2429–47