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A scaling method for asymptotic analysis of power series

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Abstract. A new method is proposed for asymptotic analysis of power series. In the method we use the relation that an n-term power series of a singular quantity with critical exponent β behaves asymptotically like $n^{-\beta}$ at the phase transition point. The method is tested on known series with satisfactory results and used to analyse the power series of the two-dimensional three-state Potts model of Enting, in good agreement with den Nijs' conjecture.

1. Introduction

The series expansion methods are some of the most powerful tools for investigating phase transitions in different physical systems (for a review see Domb and Green 1974). To determine the different series (high and low temperature, density, strong and weak coupling, $1/N$, etc) several effective methods have been developed (Domb and Green 1974, Nickel 1981) and also many powerful procedures are known for their asymptotic analysis (for a review see Gaunt and Guttmann 1974). The common feature of these analysing methods (ratio method, Padé approximants, N-point fits, etc) is that the properties of the singularity are determined from the behaviour of the power series in the vicinity of the singularity point.

In this paper we propose a new method, which concentrates on the properties of the series just at the phase transition point. It is easy to show that in nth order of the expansion a singular quantity characterised by a β critical exponent at the phase transition point asymptotically behaves as $n^{-\beta}$. This relation is used in this paper to develop a procedure for asymptotic analysis of power series. The method in some respects is analogous to finite-size scaling (for a review see Barber 1983), since by the latter method the scaling form of a physical quantity at the phase transition point as a function of the linear size of the system is used to determine the critical parameters.

The layout of the paper is as follows. Section 2 contains the description of the method, while in § 3 several power series are analysed. To test the accuracy of the method the magnetisation, the specific heat and the susceptibility series of the one-dimensional transverse Ising model (TIM) at $T = 0$ and that of the two-dimensional Ising model are analysed. As a further application, the magnetisation and the specific heat series of the two-dimensional three-state Potts model (Enting 1980) is evaluated and found to be in much better agreement with den Nijs' (1979) conjecture, compared with previous estimates. Finally, § 4 contains a short discussion and a comparison is given with other methods.

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2. Description of the method

Let the physical quantity $M = M(x)$ have a power law singularity at $x = x_0$, the phase transition point:

$$M(x) = A\left(1-\frac{x}{x_0}\right)^{\beta}\left[1+b_1\left(1-\frac{x}{x_0}\right)^{\delta}+\ldots\right] \qquad (x \to x_0). \tag{2.1}$$

(In the following we have $\beta \geqslant 0$, and for $\beta < 0$ the inverse of $M(x)$ is taken.) Furthermore, suppose that there exists the power series of $M(x)$ in the vicinity of $x = 0$:

$$M(x) = A \sum_{i=0}^{\infty} a_i \left(\frac{x}{x_0}\right)^i. \tag{2.2}$$

For large values of i the a_i coefficients can be approximated by the

$$\binom{\beta}{i} = \frac{\beta(\beta-1)\ldots(\beta-i+1)}{i!} \tag{2.3}$$

binomial coefficients, which may be expressed as (Luke 1975)

$$\binom{\beta}{i} = \frac{(-1)^i i^{-(\beta+1)}}{\Gamma(-\beta)}\left[1+\frac{\beta(\beta+1)}{2i}+O\left(\frac{1}{i^2}\right)\right] \tag{2.4}$$

where $\Gamma(x)$ is the gamma function.

Now let us form the nth partial sum of the $M(x)$ quantity:

$$M^{(n)}(x) = A \sum_{i=0}^{n} a_i \left(\frac{x}{x_0}\right)^i. \tag{2.5}$$

Obviously,

$$\lim_{n\to\infty} M^{(n)}(x) = \begin{cases} 0 & \text{if } x = x_0 \\ \text{finite} & \text{otherwise.} \end{cases} \tag{2.6}$$

(If $M(x)$ is the magnetisation, then $\lim_{n\to\infty} M^{(n)}(x) = 0$ for $x \geqslant x_0$.) Using equation (2.4) the asymptotic form of $M^{(n)}(x_0)$ can be determined at the phase transition point:

$$M^{(n)}(x_0) = A\frac{n^{-\beta}}{\Gamma(1-\beta)}\left[1-\frac{\beta}{n}(b(\beta)+B(n))+O\left(\frac{1}{n^{1+\delta}}\right)\right]. \tag{2.7}$$

Here $b(\beta) = (1-\beta)/2$, and $B(n)$ is related to the form of the confluent singularity:

$$B(n) = b_1 n^{1-\delta}\frac{\Gamma(1-\beta)}{-\beta\Gamma(1-\beta-\delta)}. \tag{2.8}$$

When the confluent singularity is additive, i.e. $\delta = 1$, then $B(n) = b_1$ and it is possible to arrange $M^{(n)}(x_0)$ in a series with integer powers of n^{-1}.

From the practical point of view it is useful to make the expression (2.7) continuous by a $\Delta(n)$ shift in the n variable:

$$M^{(n)}(x_0) = \frac{A}{\Gamma(1-\beta)}(n+\Delta(n))^{-\beta[1+n^{-1}(b(\beta)+B(n)-\Delta(n))]}\left[1+O\left(\frac{1}{n^{1+\delta}}\right)\right]. \tag{2.9}$$

(Strictly speaking, in the exponent of this expression a factor $(n \log n)^{-1}$ appears instead of n^{-1}. However, the two expressions give practically the same results, even for moderately large values of n.) According to equation (2.9) the log $M^{(n)}(x_0)$ against $\log(n+\Delta(n))$ plot is asymptotically a line with slope β. Furthermore, the mean deviation of the points from the line is the least when the coefficient of the $1/n$ term vanishes:

$$b(\beta)+B(n)-\Delta(n)=0. \tag{2.10}$$

The relation (2.9) is true for relatively small values of n, as is seen in figure 1, where the latent heat of the TIM is plotted. (The series of the latent heat in this case is defined as the difference of the slopes of the strong and weak coupling series for the ground state energy at the phase transition point (see equation (3.4).) In this simple case, when the confluent singularity is additive, so are the points, even for $n \geqslant 2$ fairly close to the

$$-\log L^{(n)}=\log \pi+\log(n+\tfrac{1}{4}) \tag{2.11}$$

line, which describes the exact asymptotic behaviour (Pfeuty 1970, Iglói *et al* 1986). From the expression (2.11) one can read $\beta=1-\alpha=1$; thus the specific heat exponent $\alpha=0$.

In the following, by making use of equation (2.9), we propose a procedure to obtain quantitative results for the critical parameters. Suppose that the first N terms of the (2.5) series are known and $1 \leqslant n_1 \leqslant n_2 \leqslant N$. Then the following expressions are defined:

$$\tilde{\beta}(n, \Delta(n))=\frac{\log M^{(n)}-\log M^{(n+1)}}{\log(n+1+\Delta(n))-\log(n+\Delta(n))} \tag{2.12}$$

where $n=n_1, n_1+1, \ldots, n_2-1$. (In some cases it is useful to compare the odd and even partial sums separately.) In the next step a $\beta(n_1, n_2)+n^{-1}\gamma(\Delta(n_1, n_2))$ line is fitted to the $\tilde{\beta}(n, \Delta(n))$ points by the least squares method. The value of $\Delta(n_1, n_2)$ is fixed by the requirement $\gamma(\Delta^*(n_1, n_2))=0$. This equation allows us to determine the form of the confluent singularity through equations (2.8) and (2.10). The critical

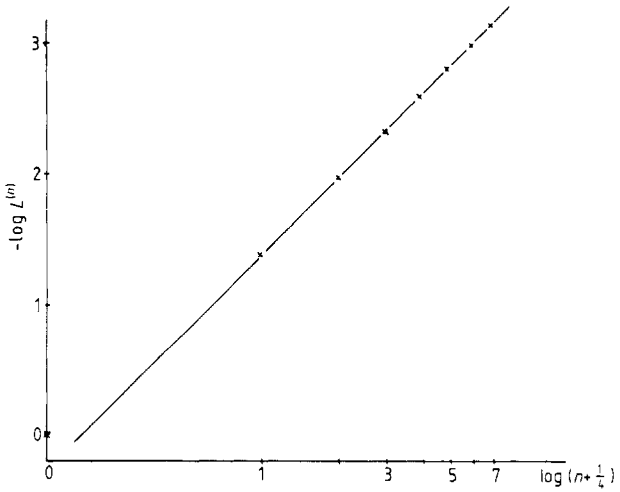

Figure 1. A log $L^{(n)}$ against $\log(n+\frac{1}{4})$ plot for the TIM. The full line represents the exact asymptotic behaviour given by equation (2.11).

exponents obtained in this way only slightly depend on n_1 and n_2, and generally the following relation applies:

$$|\beta(n_1, n_2) - \beta| \approx \frac{c}{(n_1 n_2)^{(1+\delta)/2}} \tag{2.13}$$

where $c/\beta \ll 1$. In the next section this method is used to evaluate some power series.

3. Application of the method

In this section the method is first tested on known series, and then the low temperature expansion for the two-dimensional three-state Potts model (Enting 1980) is analysed.

The magnetisation expression for the TIM is a simple power law (Pfeuty 1970, Hamer and Kogut 1979):

$$M = (1 - x^{-2})^{1/8}. \tag{3.1}$$

Therefore the ratio method predicts the exact critical parameters: $x_0 = 1$, $\beta = \frac{1}{8}$. The results of the scaling method for $x_0^2 = 1$, $x_0^2 = 1.001$ and $x_0^2 = 0.999$ are given in table 1

Table 1. Estimated values for the magnetisation exponent of the TIM.

(*a*) At the critical point $x_0^2 = 1$.

	n_2						
n_1	2	3	4	5	6	7	8
1	0.126 76	0.126 44	0.126 22	0.126 07	0.125 95	0.125 86	0.125 79
2		0.125 88	0.125 73	0.125 63	0.125 56	0.125 50	0.125 46
3			0.125 52	0.125 45	0.125 39	0.125 35	0.125 32
4				0.125 35	0.125 30	0.125 27	0.125 24
5					0.125 25	0.125 22	0.125 20
6						0.125 19	0.125 17
7							0.125 14

(*b*) At $x_0^2 = 1.001$.

1	0.125 38	0.124 85	0.124 44	0.124 09	0.123 79	0.123 51	0.123 26
2		0.123 93	0.123 56	0.123 25	0.122 96	0.122 70	0.122 45
3			0.123 02	0.122 71	0.122 43	0.122 16	0.121 91
4				0.122 29	0.122 00	0.121 73	0.121 48
5					0.121 64	0.121 36	0.121 10
6						0.121 03	0.120 76
7							0.120 44

(*c*) At $x_0^2 = 0.999$.

1	0.128 16	0.128 05	0.128 04	0.128 09	0.128 17	0.128 27	0.128 38
2		0.127 86	0.127 95	0.128 08	0.128 23	0.128 39	0.128 55
3			0.128 09	0.128 27	0.128 45	0.128 65	0.128 84
4				0.128 50	0.128 72	0.128 94	0.129 16
5					0.129 00	0.129 23	0.129 47
6						0.129 53	0.129 78
7							0.130 09

for $N = 8$. It is easily seen that at the critical point, even for this short series, the calculated $\beta(n_1, n_2)$ values are close to the exact value, and relation (2.13) is also applicable with $c \approx 0.01$. Repeating the calculation by one thousand, far from the critical point, as is seen in table 1, the $\beta(n_1, n_2)$ values vary quickly with increasing n_1 and n_2; they tend to zero above the critical point and tend to infinity below it. By this method, from this short series, the critical point and the critical exponent may be estimated within errors 0.0001 and 0.001, respectively.

For the next example the specific heat exponent of the TIM is evaluated. The strong coupling series for the ground state energy is exactly known (Pfeuty 1970, Iglói *et al* 1986):

$$E_0 = -\sum_{i=0}^{\infty} a_i (x^{-2})^i \tag{3.2}$$

where

$$a_i = \prod_{k=1}^{i} \left(\frac{2k-3}{2k}\right)^2 \qquad i = 1, 2, \ldots \tag{3.3}$$

$$a_0 = 1.$$

The specific heat exponent is determined from the series of the latent heat (Iglói *et al* 1986):

$$L^{(n)} = \sum_{i=0}^{n} (4i-1) a_i x^{-2i} \tag{3.4}$$

using the fact that $L(x) \propto x^{1-\alpha}$ in the vicinity of the critical point. The calculated $1-\alpha = \beta(n_1, n_2)$ exponents are given in table 2 for $N = 7$. Now the critical exponent may be estimated within 0.001 error. Furthermore, $b_1 = 0.25 \pm 0.01$ is found to be in good agreement with the exact value of the strength of the additive confluent singularity: $b_1 = \frac{1}{4}$.

The susceptibility series of the TIM is not known exactly and therefore the eight-term series of Hamer and Kogut (1979) is used in the analysis. The odd and even terms of this series behave differently; therefore we compare these separately. The calculated values, given in table 3, also show oscillation. Thus the γ exponent can be estimated with a relatively larger error: $\gamma = 1.75 \pm 0.005$.

Table 2. Estimated values for the $1-\alpha$ exponent of the TIM at the critical point. The exact value is $\alpha = 0$.

	n_2					
n_1	2	3	4	5	6	7
1	1.012 72	1.010 30	1.008 71	1.007 58	1.006 73	1.006 07
2		1.006 00	1.004 99	1.004 29	1.003 77	1.003 38
3			1.003 49	1.002 98	1.002 60	1.002 32
4				1.002 28	1.001 98	1.001 76
5					1.001 61	1.001 42
6						1.001 19

Table 3. Estimated values for the susceptibility exponent of the TIM at the critical point. The exact value is $\gamma = 1.75$.

	n_2				
n_1	3	4	5	6	7
1	1.7530	1.7437	1.7434	1.7430	1.7434
2		1.7287	1.7369	1.7391	1.7408
3			1.7490	1.7458	1.7460
4				1.7416	1.7446
5					1.7483

To analyse high and low temperature series we choose as test examples the magnetisation, the internal energy and the susceptibility series of the two-dimensional square lattice Ising model:

$$M = 1 - \sum_{i=1}^{\infty} b_i u^i$$
$$U = \sum_{i=1}^{\infty} c_i u^i \tag{3.5}$$
$$\chi = 1 + \sum_{i=1}^{\infty} a_i u^i.$$

Here, due to self-duality, u may be a high temperature ($u = \tanh(\beta J)$) or low temperature ($u = \exp(-2\beta J)$) expansion parameter. The coefficients of these series are taken from the review article of Domb (1974) and the specific heat exponent is calculated from the relation

$$U(u) - U(u_0) \propto \left(1 - \frac{u}{u_0}\right)^{1-\alpha} \tag{3.6}$$

where $U(u_0) = -\sqrt{2}$ (Domb 1974).

The calculated $\beta(n_1, N)$ values for $2 \leq n_1 \leq N-1$ are given in table 4, where for the latent heat and the susceptibility series the $n_1[\beta(n_1, N) - \beta_{\text{exact}}]$ quantity is also given in parentheses. It is easily seen that the magnetisation and the specific heat exponents obtained by the scaling method are very accurate, as may be found by other methods (Gaunt and Guttmann 1974), but the susceptibility series is less regular. Therefore the accuracy of the estimation in this case is smaller.

Finally the low temperature series of the partition function and the order parameter (magnetisation) of the two-dimensional three-state Potts model (Enting 1980) is analysed. The specific heat exponent in this case is also determined from the internal energy series by using equation (3.6) with $U(u_0) = -(1 - 3^{-1/2})$ (Kihara *et al* 1954).

These series are non-regular and oscillatory. Therefore the calculated $1 - \alpha(n_1, N)$ and $\beta(n_1, N)$ values, given in the first column of tables 5 and 6, respectively, also show large oscillations. These large deviations can be decreased if the following averaged quantities are used in the (2.12) relation:

$$\tilde{\beta}_1(n, \Delta) = \tfrac{1}{3}[\tilde{\beta}(n-1, \Delta) + \tilde{\beta}(n, \Delta) + \tilde{\beta}(n+1, \Delta)] \tag{3.7}$$

and

$$\tilde{\beta}_2(n, \Delta) = \tfrac{1}{3}[\tilde{\beta}_1(n-1, \Delta) + \tilde{\beta}_1(n, \Delta) + \tilde{\beta}_1(n+1, \Delta)]. \tag{3.8}$$

Table 4. The $\beta(n_1, N)$ estimates for the magnetisation, the $1-\alpha$, and the susceptibility exponents of the square lattice Ising model. The exact values of the exponents are the same as those of the TIM. The $n_1[\beta(n_1, N)-\beta_{exact}]$ quantities are given in parentheses.

n_1	Magnetisation	Latent heat	Susceptibility
2	0.124 83	0.9923 (0.0155)	1.7274 (0.0452)
3	0.124 87	0.9927 (0.0219)	1.7350 (0.0450)
4	0.124 90	0.9952 (0.0192)	1.7375 (0.0501)
5	0.124 92	0.9966 (0.0172)	1.7398 (0.0508)
6	0.124 93	0.9974 (0.0155)	1.7408 (0.0552)
7	0.124 94	0.9979 (0.0145)	1.7422 (0.0548)
8	0.124 94	0.9983 (0.0138)	1.7428 (0.0575)
9	0.124 95	0.9985 (0.0133)	1.7436 (0.0575)
10	0.124 95	0.9987 (0.0130)	1.7441 (0.0593)
11	0.124 96	0.9988 (0.0127)	1.7446 (0.0593)
12	0.124 96	0.9990 (0.0125)	1.7449 (0.0610)
13	0.124 96	0.9991 (0.0123)	1.7453 (0.0607)
14	0.124 97	0.9991 (0.0122)	1.7455 (0.0626)
15	0.124 97	0.9992 (0.0121)	1.7459 (0.0618)
16	0.124 97	0.9993 (0.0119)	1.7460 (0.0646)
17	0.124 97	0.9993 (0.0118)	1.7463 (0.0626)
18	0.124 97		1.7460 (0.0716)
19	0.124 98		
Exact	0.125	1.0	1.75

Table 5. Estimates for the $1-\alpha$ exponent of the two-dimensional three-state Potts model. The values in the second and third columns were calculated by using the averages in equations (3.7) and (3.8), respectively. The last row contains the averages of the values in rows 11-23.

n_1	$1-\alpha(n_1, N)$	$1-\alpha_1(n_1, N)$	$1-\alpha_2(n_1, N)$
11	0.6796	0.6726	0.6732
12	0.6734	0.6659	0.6700
13	0.6518	0.6668	0.6689
14	0.6881	0.6674	0.6667
15	0.6497	0.6596	0.6648
16	0.6715	0.6683	0.6650
17	0.6823	0.6635	0.6634
18	0.6468	0.6655	0.6660
19	0.6932	0.6710	0.6664
20	0.6558	0.6607	0.6662
21	0.6634	0.6710	0.6683
22	0.6949	0.6649	0.6655
23	0.6368	0.6618	0.6677
24	0.7006	0.6733	0.6670
25	0.6669	0.6537	0.6645
26	0.6322	0.6673	0.6691
Average	0.6682	0.6661	0.6671

Table 6. Estimates for the magnetisation exponent of the two-dimensional three-state Potts model. The values in the second and third columns were calculated in the same way as in table 5.

n_1	$\beta(n_1, N)$	$\beta_1(n_1, N)$	$\beta_2(n_1, N)$
11	0.1105	0.1097	0.1093
12	0.1107	0.1093	0.1094
13	0.1077	0.1095	0.1095
14	0.1125	0.1100	0.1095
15	0.1079	0.1091	0.1095
16	0.1103	0.1102	0.1097
17	0.1108	0.1094	0.1095
18	0.1081	0.1097	0.1098
19	0.1117	0.1101	0.1097
20	0.1090	0.1093	0.1097
21	0.1095	0.1101	0.1099
22	0.1119	0.1097	0.1097
23	0.1076	0.1095	0.1099
24	0.1122	0.1104	0.1099
25	0.1098	0.1089	0.1097
26	0.1077	0.1101	0.1101
27	0.1178	0.1095	0.1095

The calculated exponents now behave more regularly, as is seen from the results given in the second and third columns of tables 5 and 6. The $1-\alpha(n_1, N)$ values do not show a systematic trend with n_1. Therefore their average is a reasonable estimate for the critical exponent:

$$\alpha = 0.333 \pm 0.004. \tag{3.9}$$

The calculated magnetisation exponents $\beta(n_1, N)$ show smaller deviations, but they are systematically increasing with n_1. The estimated value is

$$\beta = 0.1105 \pm 0.001. \tag{3.10}$$

These estimates for the α and β exponents are in excellent agreement with den Nijs' (1979) conjecture: $\alpha = \frac{1}{3}$ and $\beta = \frac{1}{9}$. We note that earlier analysis of these series by other methods predicted far less accurate exponents (Enting 1980, Zwanzig and Ramshaw 1977, Miyashita *et al* 1979).

4. Discussion

In this paper a scaling method is proposed for asymptotic analysis of power series. According to the basic equation (2.7) of the method, the estimate for the critical exponent in the nth step is

$$\beta_s^{(n)} = -\frac{\log M^{(n)} - \log M^{(n-1)}}{\log n - \log(n-1)} \tag{4.1}$$

which can be written for large n as

$$\beta_s^{(n)} \approx -\frac{\delta \log M(n)}{\delta \log n}. \tag{4.2}$$

The same quantity in the ratio method (Gaunt and Guttmann 1974) is

$$\beta_{\rm r}^{(n)} = n\left(1 - \frac{M^{(n)} - M^{(n-1)}}{M^{(n-1)} - M^{(n-2)}}\right) - 1. \tag{4.3}$$

This behaves for large n as

$$\beta_{\rm r}^{(n)} \approx -\frac{\delta \log(\delta M(n)/\delta n)}{\delta \log n} - 1. \tag{4.4}$$

In the case of the $D \log$ Padé approximation (Gaunt and Guttmann 1974) we have

$$\beta_{\rm p}^{(n)} = \lim_{x \to x_0} \frac{\delta \log M^{(n)}(x)}{\delta \log(x_0 - x)}. \tag{4.5}$$

Now supposing that $M^{(n)}(x_0) = M(x_n)$, and x_n satisfies $x_0 - x_n \sim n^{-1}$, then

$$\beta_{\rm p}^{(n)} \approx -\frac{\delta \log M(n)}{\delta \log n}. \tag{4.6}$$

Comparing (4.2), (4.4) and (4.6) one can conclude that the scaling method is related to the $D \log$ Padé method. Both methods determine the critical exponents from the first derivative of the series, while the ratio method uses the second derivative.

To compare the accuracy of the scaling method with other procedures some standard trial series with known singularities (Hunter and Baker 1973) are analysed. These series are given in table 7. Following Hunter and Baker (1973), the parameter

$$\varepsilon_n = -\log_{10}\left(\frac{\Delta\beta_n}{\beta_{\rm exact}}\right) \tag{4.7}$$

by which an estimate of the critical exponent using n terms of the series is determined, where $\Delta\beta_n$ is the amount by which the series differs from the exact value $\beta_{\rm exact}$. The results of the calculation are summarised in table 8, for $n = 10$, 15, 20, together with those obtained by Hunter and Baker (1973) by other methods. It is seen that the accuracy of the scaling method for these series is comparable with the $D \log$ Padé analysis and generally superior to the ratio method. Concerning the problem of the analysis of a series with logarithmic confluent singularity (series L), we can say that the scaling method is also unable to give a reasonable estimate for the critical exponent. However, the type of the confluent singularity may be accurately determined.

Finally we may conclude that the scaling method can be applied with success for oscillating non-regular series, as was shown in the example of the three-state Potts model. Another promising field is the analysis of series where the coefficients contain some noise. The uncertainties on the coefficients make the analysis more difficult by standard methods, but by taking partial sums these uncertainties are somehow washed out (Dekeyser 1985). Another important field of application of the method seems to be the first-order transitions, which is discussed in a separate paper (Iglói *et al* 1986).

Table 7. Functions given by Hunter and Baker (1973) used in this paper to study the relative accuracy of the scaling method.

C	$(1-x)^{-1.5}(1-\frac{1}{2}x)^{1.5} + e^{-x}$
G	$(1-x)^{-1.5} + \{2(1-x)(2-x)^6/[(2-x)^7 - x^7]\}^{1.25}$
K	$(1-x)^{-1.5} + (1+\frac{4}{3}x)^{-1.25} + e^{-x}$
L	$-(1-x)^{-1.5}\ln(1-x)$

Table 8. The relative accuracy of the scaling method (S) compared with the results obtained (Hunter and Baker 1973) by the ratio method (R), Neville extrapolation (N) and Padé approximants (P). The parameter ε_n given by equation (4.7) is tabulated for $n = 10, 15, 20$.

Series	Number of terms	S	R	N	P
	10	2.2	1.3	1.8	1.7
C	15	2.6	1.5	3.6	2.4
	20	3.0	1.6	5.4	3.1
	10	1.2	1.3		0.8
G	15	1.5	1.4		1.1
	20	2.4	1.5		2.0
	10	1.6	0.7		1.4
K	15	1.9	1.2		2.0
	20	2.5	1.4		2.5
	10	0.8	0.5	0.8	0.8
L	15	0.8	0.6	0.9	0.9
	20	0.9	0.7	0.9	0.9

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