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Bayesian analysis of series expansions

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Abstract

Since the ground-breaking work of Baker and others, the analysis of series expansions using Padé approximants has been an essential technique for calculating critical properties. In this paper, we present a new approach to the analysis of series expansions based on a Bayesian analysis of the information contained in the series. This new method is capable of determining critical properties with greatly improved accuracy.

1. Introduction

The analysis of series expansions was perhaps the earliest approach to the accurate calculation of critical exponents in the theory of phase transitions. With the advent of computers, it became possible to generate expansions of the partition function or the magnetic susceptibility in powers of the inverse temperature or magnetic field [1]. The coefficients of the leading terms can be obtained exactly for various models of interest, with the number of such terms ranging from six to fifty. The task was then to extract the information about the locations and exponents of critical singularities contained in those coefficients.

The Padé approximant method [2,3] is the best known of a variety of numerical methods that have been developed for this task, although Neville tables [2], differential approximants [2], and other methods have also proven useful. The results have been very good, with the determination of up to three or four significant digits in the critical exponents [1].

Despite their achievements, Padé approximants and the other standard methods have three problems. First, their convergence properties have never been completely understood, and they give results not accompanied by reliable error analysis. Second, these methods exhibit steeply diminishing returns: after a certain point, the inclusion of more terms in the series expansions tends to produce relatively little improvement, even though an enormous computational effort is required to calculate each additional coefficient. Third, certain types of non-analytic behavior, such as confluent singularities and logarithmic corrections, have proven particularly difficult to deal with. This is especially serious since all critical phenomena involve confluent singularities as corrections to scaling.

In this paper, we present a new method for analyzing series expansions that overcomes many of these problems. The method differs qualitatively from standard approaches in that it produces a Bayesian probability distribution to describe the information about the parameters of interest that is contained in the known coefficients [4]. The width of this probability distribution provides an estimate of the uncertainty in the calculation.

A unique consequence of the Bayesian approach is that all available information concerning the critical properties of the system can be incorporated explicitly into the calculation, whether the information comes from duality conditions, finite-size scaling of Monte

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Carlo data, or Monte Carlo renormalization group calculations. It is also possible to combine the information from two or more series in a straightforward manner.

2. Method

Any particular function $F(x)$ has a power series expansion about 0 whose nth order coefficient is a_n. Given the first N coefficients of this series, the goal is to determine location of a singularity (the critical temperature) and the value of the exponents of that singularity.

Bayesian analysis is based on interpreting "probability" as a description of the knowledge of the investigator, instead of the more usual (in physics) interpretation in terms of frequency of occurrence of an event [4]. The analysis begins with Bayes' Theorem,

$$P(\theta|X) = P(X|\theta)P(\theta)/P(X), \tag{1}$$

where θ indicates the set of parameters to be determined (critical temperature, critical exponents, etc.), and X indicates the set of experimental data. $P(\theta|X)$ is the conditional probability distribution of the parameters θ, given the experimental results, X. $P(X|\theta)$ is known as the likelihood and is the conditional probability of X given θ, viewed as a function of θ. $P(\theta)$, called the prior distribution, represents our knowledge of the parameters before we include the experimental results X.

Although "data" in Bayesian analysis usually refers to experimental results with accompanying experimental errors, we have extended the concept of data to have X represent the leading series expansion coefficients, which can be calculated exactly. Since there are no errors in the data, this produces a singular likelihood, which is rather unusual in Bayesian analysis.

Our analysis exploits the fact that we know a great deal about the functions we are investigating. Our first assumption is that the function can be represented as a sum of non-analytic terms plus an analytic remainder. As an initial approximation, these non-analytic terms can be a sum of singularities, although the analysis can be extended to products of singularities, logarithmic corrections, etc.

$$F(x) = \sum_{m=0}^{\infty} A_m (1 - y_m x)^{\alpha_m} + f(x). \tag{2}$$

The assumption that $f(x)$ is analytic is expressed in terms of the coefficients of its series expansion, f_n. We assume that the magnitudes of the coefficients f_n decrease with n, and can be described by a distribution

$$f_n \sim N\big(0, (Bs^n/n!)^2\big). \tag{3}$$

An example of an analytic function that satisfies this assumption would be $B\exp(sx)$. We have assumed that B and s are independent and both are distributed exponentially, so that, for example,

$$P(B) = (1/B_0)\exp(-B/B_0), \quad B \geqslant 0. \tag{4}$$

We have found that the results are only very weakly dependent on the values we choose for B_0 and s_0, and we have usually chosen $B_0 = s_0 = 1$.

To write the likelihood explicitly, we expand the singularities in Eq. (2) to obtain

$$\sum_{m=0}^{\infty} A_m (1 - y_m x)^{\alpha_m} = \sum_{n=0}^{\infty} d_n x^n, \tag{5}$$

where the set $\{d_n\}$ is a function of the set of parameters $\{A_m, y_m, \alpha_m\}$. The likelihood is then given by the simple form

$$P(X|\theta) = \prod_{n=0}^{\infty} \delta\big(a_n - (d_n + f_n)\big), \tag{6}$$

where δ is the Dirac delta function. Finally, we include any information that we have about the theoretical parameters θ. In most of the tests we have carried out, we have assumed very broad Gaussian distributions for all of the parameters being investigated, so that the results were not greatly influenced by variations in these assumptions. We also investigated the effect of locking certain known parameters, like the location of the phase transition in the $d = 2$ Ising model, to the correct values.

3. Test series

To demonstrate the Bayesian method, we present results for three test series, along with a comparison with the Padé approximant method. The first test series is a simple branch point plus an exponential function,

$$F_1(x) = (1 - x)^{-3/2} + \exp(-x). \tag{7}$$

Table 1 shows the results of the usual Padé analysis of the logarithmic derivative of $F_1(x)$. For simplicity,

Table 1
Padé results for $F_1(x)$

Order	[N, D]	Location	Exponent
17	[8,8]	1.00002	1.5018
19	[9,9]	0.99996	1.4963
21	[10,10]	1.000007	1.50092
23	[11,11]	0.999996	1.49969
25	[12,12]	1.0000030	1.50053
27	[13,13]	1.0000022	1.50044
29	[14,14]	1.0000014	1.50033
31	[15,15]	1.0000007	1.50022
Exact		1	1.5

only the diagonal terms in the Padé table have been shown. The usual notation [N, D] has been used, with N giving the order of the numerator of the Padé approximant and D giving the order of the denominator. Including the term lost in the differentiation, the [N, D] Padé result requires the original series to order $N + D + 1$. Table 1 uses between 17 and 31 terms. The Padé results for this simple example are very good, finding 7 significant digits for the location of the singularity and 4 for the exponent.

Instead of a Padé table, our method only produces one result, a probability distribution, for a given number of terms. The values given are the values of y and γ at the maximum of the probability distribution. Table 2 shows the Bayesian results for the same function, $F_1(x)$. The error estimates are standard deviations of the probability distribution, obtained from the second derivative. The deviation from the exact answer is usually within two or three standard deviations. Table 2 uses between 10 and 15 terms in the series. No logarithmic derivative is performed, so the amplitude of the singularity is determined as part of the calculation. The Bayesian results have an unprecedented accuracy. It should be noted that the highest order series used in Table 2 is 15, where the lowest order series used in Table 1 was 17.

Tables 3 and 4 show the Padé and Bayesian results for the more difficult case of confluent singularities, again with an added analytic term,

$$F_2(x) = (1-x)^{-3/2} + (1-x)^{-9/10} + \exp(-x). \quad (8)$$

The Padé results in Table 3 give only the leading singularity. The location of the singularity is rather well determined, but the value of the exponent is somewhat low. The Bayesian results in Table 4 give

Table 2
Bayesian analysis results for $F_1(x)$ where form of singularity is $A(1-yx)^{-\gamma}$

Order	y	γ
10	1.0006(4)	1.4994(5)
11	0.999993(5)	1.50008(6)
12	1.0000008(5)	1.499991(7)
13	0.99999993(5)	1.5000010(7)
14	1.000000006(5)	1.49999991(7)
15	0.9999999995(4)	1.500000008(6)
Exact	1	1.5

Table 3
Padé results for $F_2(x)$

Order	[N, D]	Location	Leading exponent
17	[8,8]	0.99978	1.4589
19	[9,9]	0.99975	1.4570
21	[10,10]	0.99985	1.4643
23	[11,11]	0.999989	1.4685
25	[12,12]	0.999918	1.4717
27	[13,13]	0.999940	1.4749
29	[14,14]	0.999960	1.4783
31	[15,15]	0.999959	1.4782
Exact		1	1.5

Table 4
Bayesian analysis results for $F_2(x)$ where form of singularity is $A(1-yx)^{-\gamma_1} + B(1-yx)^{-\gamma_2}$

Order	y	γ_1	γ_2
13	0.9997(2)	1.523(14)	0.96(3)
14	1.00003(2)	1.497(2)	0.890(6)
15	0.999996(2)	1.5004(2)	0.9013(7)
16	1.0000004(2)	1.49996(3)	0.89985(10)
17	0.99999996(2)	1.500004(3)	0.900016(10)
18	1.000000003(2)	1.4999996(3)	0.8999985(10)
19	0.9999999997(2)	1.50000003(2)	0.90000013(9)
20	1.00000000002(1)	1.499999998(2)	0.899999990(7)
Exact	1	1.5	0.9

Table 5
Padé and Bayesian analysis results for $F_3(x)$ where form of singularity for Bayesian analysis is $A(1-yx)^{-\gamma}[1-b\ln(1-yx)]$

Padé results			Bayesian analysis results		
Order	[N,D]	Exponent	Order	γ	Ab, amplitude of log
17	[8,8]	1.7112	10	1.485(9)	0.95(3)
19	[9,9]	1.6907	11	1.503(2)	1.009(5)
21	[10,10]	1.6945	12	1.4996(2)	0.9986(9)
23	[11,11]	1.6848	13	1.50004(3)	1.00018(12)
25	[12,12]	1.6787	14	1.499995(3)	0.999978(115)
27	[13,13]	1.6736	15	1.5000005(4)	1.0000024(16)
29	[14,14]	1.6683	16	1.49999995(3)	0.99999977(16)
31	[15,15]	1.6620	17	1.500000004(2)	1.000000021(15)
Exact		1.5	Exact	1.5	1

both singularities, with the location, exponents, and amplitudes determined very well.

The final example, shown in Table 5, uses a function that includes logarithmic corrections,

$$F_3(x) = (1-x)^{-3/2}\,(1-\ln(1-x)) + \exp(-x). \quad (9)$$

The Padé results in Table 5 show estimates for the exponent that are much too high. Even worse, it looks as if it is converging rather well to a value of about 1.66, with no hint that it is quite wrong. The Bayesian results in Table 5, on the other hand, obtain the correct value of the exponent, and the amplitude of the logarithmic correction.

4. Future work

We are currently applying the Bayesian method to the analysis of series for various models in statistical mechanics. In addition to the functions described above, we are able to investigate more than one singularity, so that both ferromagnetic and antiferromagnetic singularities are determined from the same calculation. Future work will include the analysis of low-temperature series and series in two or more variables (tricritical points) [1]. We are also able to include two or more series in the same calculation, so that we will be able to determine a universal critical exponent from series for several different lattice. As new results becomes available from any source, such as Monte Carlo simulations, the new information can be used by our method to sharpen the analysis of the related series. We believe that the method will also be useful for problems in related areas, such as lattice gauge theories for quantum chromodynamics (QCD).

References

[1] J.J. Binney, N.J. Dowrick, A.J. Fisher, M.E.J. Newman, The Theory of Critical Phenomena (Clarendon Press, 1992).
[2] D.L. Hunter, G.A. Baker, Jr., Methods of series analysis. I: Comparison of methods used in critical phenomena, Phys. Rev. B 7, 3346–3376.
[3] G.A. Baker, Jr., P. Graves-Morris, Padé Approximants, 2nd ed. (Cambridge University Press, 1996).
[4] For an introduction to Bayesian analysis, consult A.O. O'Hagan, Bayesian Inference (Halsted Press, 1994) or A. Gelman, J. Carlin, H.S. Stern, D.B. Rubin, Bayesian Data Analysis (Chapman & Hall, 1995).
[5] LiDIA-Group, LiDIA – A Library for Computational Number Theory (TH Darmstadt, 1996).