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1983 J. Phys. A: Math. Gen. 16 3097

(http://iopscience.iop.org/0305-4470/16/13/034)

J. Phys. A: Math. Gen. **16** (1983) 3097–3103. Printed in Great Britain

Tests of a method for estimating corrections to scaling from series

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Received 4 January 1983, in final form 25 April 1983

Abstract. We study a recently developed, Padé-type method of series analysis which allows for the leading confluent singularity. A number of properties are described and by applying the method to various test series some pitfalls of the technique are revealed.

In a recent series of papers (Adler *et al* 1982a, b, c, Adler and Privman 1982) a new method of series analysis for confluent singularities was proposed and applied. Confluent singularities are a subject of considerable interest owing to their importance in analysing experimental data on systems near critical points (Ahlers 1980, and references therein), and Monte Carlo simulations of critical behaviour (Stauffer 1981, Djordjevic *et al* 1982), and also because a proper treatment of them serves to reduce systematic errors present in the usual Padé approximant methods of series analysis. Recent series expansion studies include: tests of hyperscaling and of the consistency between the field-theoretic renormalisation group (RG) and series estimates of the critical exponents γ and ν in the $d=3$ Ising model (Zinn-Justin 1981, Chen *et al* 1982, Adler *et al* 1982b); removal of discrepancies between the conjectured values of γ, β and δ and several series estimates for $d=2$ percolation (Adler *et al* 1982a, c, Privman and Vagner 1982), and between the conjectured and series estimates of α, β and γ for the $d=2$, $q=3$ Potts model (Adler and Privman 1982) study of the $d=3$ self-avoiding walks (McKenzie 1979). Several methods of analysing confluent terms have been suggested (consult Adler *et al* (1982c) for a critical overview and references). In this paper we investigate further the method proposed by Adler *et al* (1982a); a number of properties are considered and by applying the method to various test series some pitfalls of the technique are revealed.

Singular behaviour close to a critical point x_c is predicted by the RG theory (Wegner 1972a, b) to be of the form

$$F(x)=c_F(x_c-x)^{-h}[1+a_{1F}(x_c-x)^{\Delta_1}+b_{1F}(x_c-x)+\ldots] \tag{1}$$

as $x\to x_c^-$, where x is a temperature-like variable, h denotes the leading critical exponent (further general powers of (x_c-x) appear in the last factor), with $\Delta_1>0$ being the first confluent exponent ($\Delta_1=-y_2/y_1$ in terms of the RG eigenexponents $y_1>0>y_2>\ldots$).

Consider estimation of h using the biased Dlog Padé method. We will assume that $x_c(T_c)$ is known exactly or that a good estimate is available and derive a truncated power series for $H(x)=(x_c-x)(F'/F)$ (from a finite number of terms in the series of $F(x)$):

$$H(x)=(x_c-x)(F'/F)=h-[a_1\Delta_1(x_c-x)^{\Delta_1}+\ldots]/[1+a_1(x_c-x)^{\Delta_1}+\ldots], \tag{2}$$

so that $H(x_c)=h$. The function $H(x)$ and the value $H(x_c)$ are estimated by calculating different Padé approximants (Baker 1975) $H^{[L,M]}(x)$. *Padé sequences are not expected to converge well at branch points, such as* x_c (the term $(x_c-x)^{\Delta_1}$ is not analytic when Δ_1 is non-integral). Numerical evidence suggests that $H^{[L,M]}(x_c)$ often deviates from the correct h (when known) by an apparently stable, small, non-zero value. (Consult Adler *et al* (1982c, ch 3) for further discussion.)

In order to treat the non-analyticity arising from the leading confluent term, Adler *et al* (1982a, b, c), following Roskies (1981), propose to transform the series for $F(x)$ to an expansion in powers of

$$y=1-(1-x/x_c)^{\Delta}, \tag{3}$$

where Δ is regarded as a variable parameter and an exact x_c value is used as an input (there are likely further features of the method studied below that arise when T_c is not known accurately, but we will not consider this case here). Then they examine Padé approximants, $G_{\Delta}^{[L,M]}(y)$, to

$$\begin{aligned}G_{\Delta}(y)&=\Delta(1-y)\,\mathrm{d}\ln F(x(y,\Delta))/\mathrm{d}y\\&=h-[\tilde{a}_1\Delta_1(1-y)^{\Delta_1/\Delta}+\ldots]/[1+\tilde{a}_1(1-y)^{\Delta_1/\Delta}+\ldots]\end{aligned} \tag{4}$$

where $\tilde{a}_1\equiv a_1x_c^{\Delta_1}$. The choice $\Delta=1$ simply reproduces the usual Dlog Padé evaluation of $h\simeq G_{\Delta=1}^{[L,M]}(1)$. Adler *et al* (1982a, b, c), however, considered a family of $\tilde{h}(\Delta)$ curves in the (Δ, h) plane, defined by

$$\tilde{h}(\Delta)=G_{\Delta}^{[L,M]}(1). \tag{5}$$

Observe that when $\Delta=\Delta_1$ the $(1-y)^{\Delta_1/\Delta}$ terms in (4) become analytic. The case $\Delta\simeq\Delta_1$ was studied by Adler *et al* (1982a). Here we examine all the possible choices of Δ which make $(1-y)^{\Delta_1/\Delta}$ analytic. These are $\Delta=\Delta_1/k$, with $k=1,2,3,\ldots$. For Δ close to Δ_1/k we may linearise $G_{\Delta}(y)$ in the difference $\Delta-\Delta_1/k$. Retaining the leading terms as $y\to1$ yields

$$G_{\Delta}(y)\simeq h+\tilde{a}_1k^2(1-y)^k\ln(1-y)(\Delta-\Delta_1/k)+\mathrm{O}((1-y)^k)+\ldots. \tag{6}$$

This result implies that the effect of the leading non-analytic contribution is to produce a small non-zero *slope* of the $\tilde{h}(\Delta)=G_{\Delta}^{[L,M]}(1)$ curves in the (Δ, h) plane. For ideal estimation of h and Δ_1, the $\tilde{h}(\Delta)$ curves should intersect with small slopes at the points $\Delta=\Delta_1/k$, $h=h_{\text{exact}}$ in the (Δ, h) plane. However, finite series effects and higher confluent terms cause deviations from this ideal situation. In the series previously studied one actually observes a region of 'convergence' of $\tilde{h}(\Delta)$ curves (with a large number of intersections) at $\Delta\simeq\Delta_1$ (corresponding to $k=1$) or no 'convergence region' at all (see Adler *et al* 1982a, b, c, Adler and Privman 1982, Privman and Vagner 1982). In some cases (Adler and Privman 1982) a 'convergent' structure was also found at $\Delta\simeq1$, and it was shown that it reflects the presence of the leading analytic confluent term proportional to b_{1F} in (1).

Note that some finite series effects are present even when the influence of the higher confluent terms is negligible. Thus suppose that the first $N+1$ coefficients of the power series for $F(x)$ are available,

$$F(x) \simeq \sum_{k=0}^{N} F_n x^n, \tag{7}$$

from which the $(N-1)$-power series for $G_\Delta(y)$ may be derived. When $\Delta \equiv \Delta_1/k$, we obtain from (4) (assuming no higher terms)

$$G_{\Delta_1/k}(y) \equiv h - \tilde{a}_1\Delta_1(1-y)^k/[1+\tilde{a}_1(1-y)^k]. \tag{8}$$

This ratio of two k-degree polynomials will be reproduced exactly by a Padé approximant when both $L \geqslant k$ and $M \geqslant k$. In most applications (Baker 1975), near-diagonal approximants are used. As a rough estimate, these will approximte $G_{\Delta_1/k}(y)$ exactly for $k = 1, 2, \ldots, k_{\max}$, where $k_{\max} < (N-1)/2$. In calculations of Adler *et al* (1982a, b, c), Adler and Privman (1982) and Privman and Vagner (1982) nine 'central' Padé approximants were chosen (rather arbitrary): $[M-2, M+2]$, $[M-1, M+1]$, $[M, M]$, $[M+1, M-1]$, $[M+2, M-2]$, $[M-2, M+1]$, $[M-1, M]$, $[M, M-1]$, $[M+1, M-2]$ for even $(N-1) \equiv 2M$ and $[M-1, M+2]$, $[M, M+1]$, $[M+1, M]$, $[M+2, M-1]$, $[M-1, M+1]$, $[M, M]$, $[M+1, M-1]$, $[M-1, M]$, $[M, M-1]$ for odd $(N-1) \equiv 2M+1$. Making such choice of Padé approximants, we may obtain a stronger criterion: all $\tilde{h}(\Delta)$ curves will intersect at $(\Delta_1/k, h_{\text{exact}})$ for $k = 1, 2, \ldots, k_{\max}$ with $k_{\max} = (N-4)/2$ (for both even and odd $(N-1)$). As an illustration of what is entailed we plot in figure 1 the $\tilde{h}(\Delta)$ curves obtained from the 12-power series ($N = 12$) for the test function

$$F(x) = (1-x)^{-1.2}[1+(1-x)^{0.8}], \tag{9}$$

so that $x_c = 1$, $h = 1.2$, $\Delta_1 = 0.8$, $a_{1F} = 1$ and no further confluent terms are present. Evidently, all nine Padé curves intersect at (Δ_1, h), $(\Delta_1/2, h)$, $(\Delta_1/3, h)$ and $(\Delta_1/4, h)$ as anticipated. However, the most interesting feature of $\tilde{h}(\Delta)$ curves is a systematic deviation from the correct h value, $h = 1.200$, when Δ is away from the analyticity points. At $\Delta = 1$ the nine approximants which we consider spread over the range (not reproduced in figure 1)

$$h = 1.189 \pm 0.002, \tag{10}$$

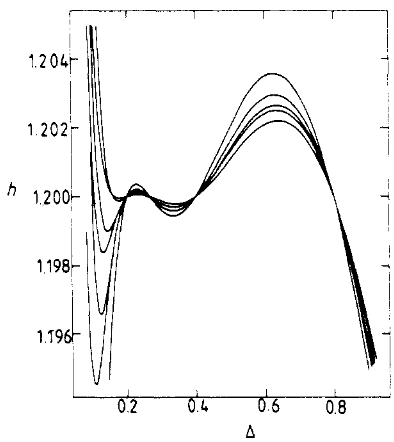

Figure 1. Curves of $\tilde{h}(\Delta)$ for the test function (9) with $h = 1.200$, $\Delta_1 = 0.8$ and no higher-order terms.

thus a (rather small) systematic error, about 1%, is present in this biased Padé estimate of h.

Higher confluent terms will complicate the pattern of $\tilde{h}(\Delta)$ curves. Consider, for example, the addition of an analytic term, as in (1), with a small amplitude b_{1F}. In figure 2 we display results for the 12-power series expansion of the test function

$$F(x) = (1-x)^{-1.2}[1+(1-x)^{0.8}+0.1(1-x)]. \tag{11}$$

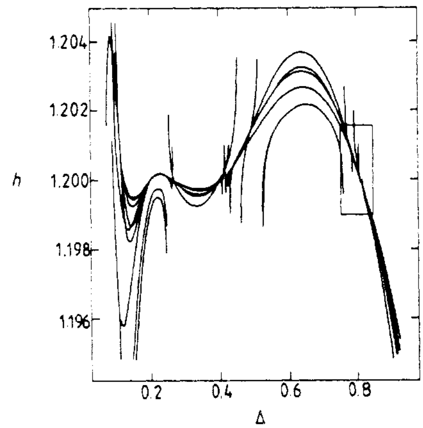

Figure 2. Curves of $\tilde{h}(\Delta)$ for the test function (11) with a 'small' ($b_{1F}/a_{1F} = 0.1$) analytic confluent term present.

The overall trend of $\tilde{h}(\Delta)$ curves in figure 2 is similar to that in figure 1, including the systematic error in h values as $\Delta \to 1$. There are, however, two new effects arising from the next-to-leading confluent terms. The first is the presence of many weak poles in the $\tilde{h}(\Delta)$ curves close to points Δ_1/k. Such poles also appeared within the $k = 1$ 'convergence region' (the only one present) in the studies of several percolation series (Adler *et al* 1982a, c) and they made the identification of the correct region more difficult. These poles probably reflect 'attempts' of Padé approximants to mimic the weak branch cuts introduced in G_Δ, see equations (4) and (8), by the higher confluent terms when superimposed on an analytic background at $\Delta \simeq \Delta_1/k$. In fact, $G_\Delta(y)$ is non-analytic away from $\Delta = \Delta_1/k$ as well. However, only when the branch cut is weak, the poles of $G_\Delta^{[L,M]}(y)$ will be very close to the branch point ($y = 1$) and presumably pass through it at some $\Delta \simeq \Delta_1/k$. The above argument is based on a numerical experience and we have no convincing 'rigorous' derivation.

The second effect of the higher terms is a distortion of the 'intersection regions'. Those with higher k are more influenced and are usually completely destroyed when a number of terms with exponents higher than Δ_1 are present, including the b_{1F} term (figure 2) and terms with other Δ_i, both integer and non-integer (this observation is based on other test-functions studies, not reported here). In all the calculations of Adler *et al* (1982a, b, c), Adler and Privman (1982) and Privman and Vagner (1982) only the $k = 1$ convergence region seemed present or there was no convergent structure at all. We have no 'rigorous' explanation of the above effect; a qualitative rationalisation is that presence of additional terms in the numerator and the denominator of $G_\Delta(y)$, equations (4) and (8), requires $G_\Delta^{[L,M]}(y)$ with higher L and M for accurate approximation, thus effectively reducing $k_{\max}$.

In figure 2 'convergence regions' with $k > 1$ have not completely disappeared. In such cases one can supplement the present method with some other method of estimating Δ_1 (see Adler *et al* 1982c for references). The $k = 1$ 'convergence region' (distorted by weak poles) is enclosed in a box in figure 2, suggesting Δ_1 and h estimates

$$h = 1.2002 \pm 0.0013, \tag{12}$$

$$\Delta_1 = 0.80 \pm 0.05. \tag{13}$$

In cases where the higher-order confluent terms have relatively large amplitudes (comparable to a_{1F}) the present method must clearly be used with caution. An instructive example is provided by the 12-power series for the test function

$$F(x) = (1-x)^{-1.2}[1 + (1-x)^{0.8} - (1-x) + 2(1-x)^{1.6}], \tag{14}$$

for which $\tilde{h}(\Delta)$ curves are plotted in figure 3. Here $b_{1F} = -1$ and a term with an exponent $2\Delta_1$, as is normally to be anticipated, and a coefficient 2 is introduced. This test function illustrates most of the problems and pitfalls possible when the leading confluent term is studied by the present method. The central ($k = 1$) 'convergence region' at $\Delta \simeq \Delta_1 = 0.8$ (A in figure 3) is cut by poles. Furthermore, even if the poles are disregarded, h estimates from this $k = 1$ region possess a residual systematic error (which is, however, less than the deviation from $h_{\text{exact}} = 1.200$ if one uses the $\tilde{h}(\Delta = 1)$ values). At $\Delta \simeq 1$ there is a 'convergence region' (B in figure 3) which may be attributed to the b_{1F} term (see Adler and Privman (1982)) and whose presence makes apparent error estimate of the usual biased Padé ($\tilde{h}(\Delta = 1)$ values) unrealistically small, since the central value is not accurate.

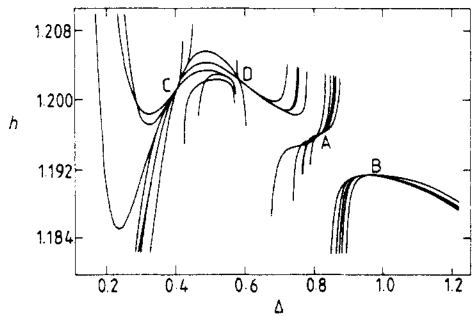

Figure 3. Curves of $\tilde{h}(\Delta)$ for the test function (14) with relatively 'large' analytic and $2\Delta_1$ confluent terms (see text).

In figure 3 only the $k = 2$ 'higher k convergence region' survived, at C ($\Delta \simeq \Delta_1/2 = 0.4$); it is well defined and happens to reproduce the correct h value. Evidently, there is a danger of making the erroneous identification $\Delta_1 \simeq 0.4$. Finally, there is some 'structure' at $\Delta \simeq 0.6$ (D in figure 3) which seems to have no obvious origin. We conclude that a complicated pattern of 'convergence regions' in the Adler *et al* (1982a) method is an indication of interfering, higher-order confluent terms. In such cases the method is certainly limited.

We do not attempt here to review other methods of single-variable series analysis of confluent singularities (see Adler *et al* 1982c). It should be noticed, however, that several known methods (Guttmann and Joyce 1972, Baker and Hunter 1973, Fisher 1977, Fisher and Kerr 1977, Hunter and Baker 1979, Fisher and Au-Yang 1979, Bessis *et al* 1980, Rehr *et al* 1980, Nickel 1981) would 'solve' all our test functions exactly (when the power series is long enough). However, an infinite sequence of higher confluent terms introduces inherent instability (Nickel 1981, see also Adler *et al* 1982c) in these methods as well.

A systematic way out of these difficulties is to employ multi-variable series expansions, in conjunction with the multi-variable first-order partial differential approximants (Chen *et al* 1982, Fisher and Chen 1981, Fisher and Styer 1982). However, multi-variable expansions require much labour, both in their derivation and analysis. Therefore, in favourable cases, especially when x_c is known, the method of Adler *et al* (1982a) may be useful; a reduction of systematic errors relative to normal Padé methods may be anticipated. Our study of various test functions reveals definite pitfalls that must be guarded against in future applications.

Acknowledgments

The author is indebted to Professor M E Fisher for his valuable comments on the manuscript. Work with Dr J Adler and Dr M Moshe on the subject of confluent singularities was most instructive and enjoyable. The support of the Rothschild Fellowship Foundation, and partial support from the National Science Foundation (through Grant No DMR-81-17011) is gratefully acknowledged.

Note added. Dr J Adler informed us recently that $k > 1$ 'convergences' are present in series analyses of several $d = 2$ problems (Adler J 1983 to be published, reported in part at the April 1983 IPS meeting).

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