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Application of the quadratic approximants to simple cubic lattice trees

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Abstract. Recent work has drawn attention to the utility of algebraic approximants for series expansion analysis. The special case of quadratic approximants are applied to lattice trees (weakly) embedded on the simple cubic lattice. The resulting estimates of x_c, the reciprocal of the growth constant, are compared with those obtained from other methods of analysis.

Series analysis of exact enumeration data has, following the pioneering work of Domb and others [1], provided accurate estimates of the critical point and exponents for a wide variety of problems in the study of phase transitions. A central difficulty of this technique is the choice of an appropriate method of analysis. In particular, the method must suit the general form of the function to be analysed.

Recent work by Brak and Guttmann [2] has drawn attention to the algebraic approximants as a method of series analysis when the critical exponent of the function to be analysed is a rational number. Quadratic approximants, a special case of algebraic approximants, are defined by the equation

$$P^{(K)}f^2 + Q^{(L)}f + R^{(M)} = 0 \tag{1}$$

where $P^{(K)}, Q^{(L)}$ and $R^{(M)}$ are polynomials of degree K, L and M respectively. The first N coefficients of the approximant f match those of the function to be approximated, with

$$N = K + L + M + 2\,. \tag{2}$$

The critical point, x_c, of a function of the form

$$F(x) = B(x) + A(x - x_c)^{1/2} \tag{3}$$

will be estimated by the zero of the determinant

$$D = {Q^{(L)}}^2 - 4P^{(K)}R^{(M)}\,. \tag{4}$$

(More specifically, x_c is here assumed to be real and positive and the zero of this type closest to the origin is used as the estimate. $B(x)$, the background term in $F(x)$, is assumed to be analytic at x_c.)

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Here quadratic approximants are applied to the generating function, G, of unrooted lattice trees weakly embedded on the simple cubic lattice

$$G = \sum_n C_n x^n \sim (x_c - x)^{-1+\theta} \tag{5}$$

($\sim$ denotes the singular part). The coefficients of this generating function to $O(x^{15})$ are available from the work of Sykes and Wilkinson [3]. Lattice trees are generally believed to be in the same universality class as lattice animals and hence it follows from the work of Parisi and Sourlas [4] that this generating function is expected to have a square root singularity of the type described by equation (3).

The results obtained from the quadratic approximants are compared with those obtained by the ratio method [5], D-log Padé approximant method [5] and the Baker–Hunter confluent singularity analysis [6, 7]. The ratio method estimates are extrapolated by means of a Neville table [5]. Methods based on Padé approximants, in general, do not provide well converged estimates of the critical point of functions with a weak singularity. Therefore, results reported here for the D-log Padé and Baker–Hunter methods are based on an analysis of the second moment of the generating function (cf [8]). (The first moment, corresponding to the rooted embeddings, was also analysed. However, convergence of the results was much poorer.)

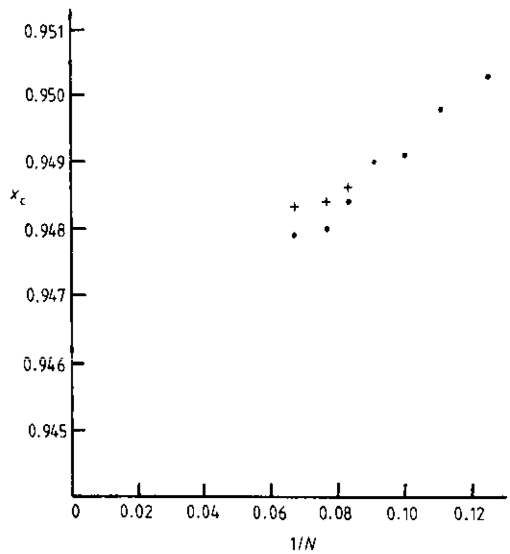

Figure 1. Variation in the estimate of x_c from the quadratic approximants with the number of coefficients fitted. Full circles represent estimates from approximants in the sequence $K = L,\ L \pm 1;\ M = L$. Crosses represent estimates from approximants in the sequences $K = L;\ M = L \pm 1$ and $K = M;\ L = M \pm 1$.

In figure 1 the estimates of x_c from various quadratic approximants are plotted against the reciprocal of the number of coefficients of the generating function matched by the approximants. The approximants corresponding to the cases

$$K = L, L \pm 1; M = L \tag{6}$$

were primarily considered (following the practice with conventional Padé approximants of considering diagonal and 'near-diagonal' entries in the Padé table). For $N \geqslant 12$, the 'near-diagonal' sequences

$$K = L; M = L \pm 1 \tag{7}$$

and

$$K = M; L = M \pm 1 \tag{8}$$

were also considered. The estimates of x_c obtained from these latter two sequences are the same (to five decimal places) when $N = 12$ and $N = 15$. However, for $N = 13$ the [4,3,4] approximant gives $x_c \approx 0.094\,84$ but the D of the [4,4,3] approximant does not have a real positive pole $\leqslant 1.0$. There appears to be a clear downward trend in the estimate of x_c as the number of terms matched increases. A reasonable linear extrapolation of this trend (figure 1), based on the last few values of x_c, would give a significant correction to the final estimate of x_c (compared with the unextrapolated values). To test for curvature in the estimates of x_c, a range-of-fit test [9] was performed using data points with $N \geqslant 8$. The [4,4,4] approximant was eliminated from the analysis as the value of x_c ($= 0.0941$) for this approximant was anomalously low compared with those from the other approximants. The results of the range-of-fit test depend strongly on the presence of the estimates of x_c from the [4,5,4] and [4,4,5] approximants. If these points (which have essentially the same value of x_c) are included, the extrapolated estimate of x_c increases as the number of data points used in the linear extrapolation decreases. This may indicate curvature in the estimates of x_c. However, if the estimates from the [4,5,4] and [4,4,5] approximants are removed, the linear extrapolants are very stable and indicate only statistical variations in the extrapolated value of x_c. While we cannot rule out curvature in the estimates of x_c, it seems likely that the estimate of x_c obtained from the [4,5,4] and [4,4,5] approximants is anomalously high and that the variation in the extrapolated x_c is an artefact of this. Consequently, the points corresponding to these approximants were removed from the analysis. The extrapolated value of x_c in table 1 was obtained from a least-squares linear fit to the remaining points and the error bounds represent the variation in the extrapolated value in the range-of-fit test.

Table 1. Estimates of x_c from the (a) quadratic approximant method (b) ratio method (c) D-log Padé approximant method and (d) Baker–Hunter confluent singularity method. The quadratic approximant value is obtained by extrapolation as described in the text. The ratio method value is based on the last few entries of the 2nd, 3rd, 4th and 5th columns of the Neville table.

	(a)	(b)	(c)	(d)
x_c	$0.094\,50 \pm 0.000\,02$	0.0946 ± 0.0002	$0.094\,87 \pm 0.000\,01$	$0.094\,81^{+0.000\,01}_{-0.000\,02}$

In table 1 we compare this extrapolated value of x_c from the quadratic approximants with the estimates of x_c obtained by other methods. The D-log Padé approximant estimate is obtained by the standard method of drawing a pole residue plot and reading the value of x_c from this plot that corresponds to the known critical exponent. In this sense this estimate is a biased one, based on the known value of the exponent, like the quadratic approximant estimate. The ratio method and the Baker–Hunter method estimates are, on the other hand, unbiased. As usual, the Baker–Hunter method estimate of x_c is obtained by performing the analysis at various trial values of x_c [7] and estimating x_c from the region of the trial values in which the real positive pole closest to the origin of the Padé approximants to the Baker–Hunter auxiliary function has its best convergence (taken over various approximants—here we use those in which the degree of the numerator and denominator differ by no more than one and the sum of the degrees is $\geqslant 10$). An estimate of θ is obtained in the Baker–Hunter analysis, by noting that the real positive pole closest to the origin of the Padé approximants is an estimate of $1/(3-\theta)$. Taking the variation in these poles over the range of the estimate of x_c we obtain

$$\theta = 1.49^{+0.02}_{-0.01} \tag{9}$$

in good agreement with the expected value.

When examining the estimates of x_c in table 1 it must be recalled that the error bounds quoted for each method reflect only the apparent convergence of the method (in the cases of the Baker–Hunter and ratio methods) or the apparent certainty with which a line may be drawn through the estimates from individual approximants (in the cases of the quadratic approximant and D-log Padé approximant methods). Moreover, the assessment of the error bounds is to some extent subjective. (Indeed, the upper bound on the Baker–Hunter estimate is slightly revised from that given in an earlier paper [10].) None the less, the discrepancy between the Baker–Hunter estimate and the quadratic approximant estimate is disquieting, especially as the trend in the quadratic approximants, already noted, tends to increase the discrepancy. Since the Baker–Hunter method, as applied here, takes into account only the scatter over various Padé approximants, we cannot altogether rule out the possibility that this is a short-series effect in the Baker–Hunter analysis. However, it prompted a consideration of possible confluences (or, in the language of critical phenomena, correction to scaling terms). The quadratic approximant method will remain valid if the confluence has an exponent which is an integer multiple of $\frac{1}{2}$. However, if this is not the case the quadratic approximants will no longer provide reasonable approximants to the generating function and we might indeed expect a systematic deviation from the true value of x_c. On the other hand, the Baker–Hunter method is applicable to any power law confluence and an estimate of the exponent of the confluence is obtained by examining the second pole on the real positive axis of the Padé approximants to the Baker–Hunter auxiliary function.

In general this second pole is not well resolved by the approximants for relatively short series. A reasonable estimate of its position may be obtained by plotting the position of the second pole as a function of the position of the first, and noting that the positions appear to be correlated for a given assumed value of x_c [11]. From a line drawn through the points on this plot an estimate of the exponent of the confluent term corresponding to the known exponent of the leading term may be obtained. This procedure was applied at the central estimate of x_c and at the extremes of the error bounds of x_c. The points corresponding to different x_cs fall on distinct lines and the variation in the estimates of the confluent exponent between lines is much greater than the uncertainty in the drawing of the lines, as might be expected.

From the above procedure, the difference between the exponent of the leading term and the confluent term—that is the correction to scaling exponent—is estimated to be

$$\Delta_1 = 0.84 \pm 0.01 \,. \tag{10}$$

Recently, Adler *et al* [12] have estimated the correction to the scaling exponent for animals using a modified Roskies transformation analysis of the data, and have reviewed earlier estimates of this quantity. The results quoted by Adler *et al* fall into two classes; those with $\Delta_1 < 1.0$ and those with $\Delta_1 \approx 1.2$. Indeed it may be noted that in the extensive analysis of Guttman and Gaunt [13] which one of these two groups the result falls into depends on the series analysed (weak or strong embeddings for example). Adler *et al* appear to dismiss the possibility of a $\Delta_1 < 1.0$, despite a good convergence in this region at $\Delta_1 \approx 0.6$, and give as their estimate $\Delta_1 = 1.3 \pm 0.2$.

The estimate of Δ_1 obtained from the Baker–Hunter analysis is consistent with the values of Guttmann and Gaunt [13] for those in the class with $\Delta_1 < 1$; however, the error bounds on the latter are quite wide. A reasonable interpretation of the result reported here, those of Guttmann and Gaunt, and that of Adler *et al*, is that two confluent terms are important and that, for at least some of the series analysed, the second confluence has a weaker singularity but a much larger coefficient than the first. Thus assuming the generating function is of the form

$$G \sim A_0(x_c - x)^{1/2}[1 + A_1(x_c - x)^{\Delta_1} + A_2(x_c - x)^{\Delta_2}] \tag{11}$$

the present results indicate the value of Δ_1 is that given above (equation (10)) and a value of $\Delta_2 \approx 1.3$ would be expected.

As already noted, the pole in the Baker–Hunter analysis corresponding to the first confluence is not well resolved. It is therefore likely that considerably longer series would be required to resolve the pole corresponding to the second confluence. Indeed, examination of the Padé approximants, used in the Baker–Hunter analysis, at the central estimate of x_c and at the extremes of the error bounds on x_c, reveals only one approximant with three real positive poles. This is the [7/7] approximant to the auxiliary function at $x_c = 0.094\,79$. The poles of this approximant estimate $\theta = 0.504$, $\Delta_1 = 0.86$ and $\Delta_2 = 1.4$. While this is consistent with the interpretation given above, results based on a single Padé approximant are, at best, very weak corroborative evidence. Margolina *et al* [14] and Lam [15] have estimated Δ_1 from an analysis of the series expansion of the radius of gyration for lattice animals on a simple cubic lattice. Margolina *et al* estimate $\Delta_1 = 0.64 \pm 0.06$ and Lam estimates $\Delta_1 = 0.45 \pm 0.01$ (the number of coefficients used by Lam was greater than those used by Margolina *et al*). However, both of these estimates are based on analyses which take into account only a single confluence. The influence of a second confluence may account for the discrepency among these estimates, and between these estimates and the value obtained above by the Baker–Hunter analysis.

In summary, a persistent trend is observed in the estimates of x_c for simple cubic lattice trees obtained by using quadratic approximants. This trend, if extrapolated, moves the estimate of x_c away from the estimate of x_c obtained by the Baker–Hunter analysis. It is probable that the trend is due to the influence of one or more confluent terms. As discussed by Brak and Guttmann [2], algebraic approximants are likely to be useful for the identification of possible exact solutions. However, as the work reported here indicates, caution must be used if applying them to obtain numerical results when the form of the function to be approximated is not known beyond the leading singularity. (This is, of course, true for any method of series analysis.)

Lastly, it may be noted that quadratic approximants may, in principal, be used to analyse singularities of the form

$$G' = (x_c - x)^{-1/2}. \tag{12}$$

In this case, x_c is estimated by the 'simultaneous' zeros of $P^{(K)}$ and $Q^{(L)}$ (and D). Numerically the zeros of these polynomials are not expected to coincide precisely except when f is the exact solution. The quadratic approximant method was therefore applied to the generating function for rooted lattice trees on the simple cubic lattice (or, equivalently, the first moment of the unrooted generating function). We find that in the sequence of approximants considered, $P^{(K)}$ and D exihibit zeros in the range [0.092, 0.095] in all cases and that the difference in these zeros for a given approximant becomes small as the number of coefficients used to form the approximant gets larger. However, for all but the highest order approximants considered ($[K = 4, L = 4, M = 4]$ and $[K = 5, L = 4, M = 4]$) $Q^{(L)}$ does not exhibit a zero in the expected region. For both of the highest order approximants $P^{(K)}$ and D exhibit zeros at $x = 0.094\,56$ and $x = 0.094\,60$ respectively with a zero in $Q^{(L)}$ at $x = 0.092\,36$. Therefore it might be expected that several more coefficients would be necessary before the required zero of $Q^{(L)}$ is sufficently close to that of $P^{(K)}$ to give any confidence in the estimate of x_c.

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