Algebraic approximants: A new method of series analysis

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Abstract

We propose a new method of series analysis in which the available series coefficients are fitted to an algebraic equation. Such a proposal restricts solutions to have algebraic singularities with rational critical exponents. The advantage of the method over the method of differential approximants is that in those cases where the two methods are exact, the algebraic approximant method usually (though not invariably) requires far fewer series coefficients for its exact specification, and hence discovery. The method is therefore potentially valuable in the study of two-dimensional critical systems in particular.

1 Introduction

In 1970, a method of series analysis was developed by Guttmann and Joyce [1]. The method was subsequently extended by others [2] and became known variously as the Recurrence Relation method, the method of Integral Approximants, and as the method of Differential Approximants (D.As.), which by now is the generally accepted title. It has become arguably the principal method of series analysis for lattice statistics models, and has been generalised by M.E. Fisher and co-workers to handle multivariate functions, in which form it is known as the method of Partial Differential Approximants (P.D.As.) [3]. The method was inspired by what were the only known exact solutions at that time, the specific heat and order parameter of the zero-field two-dimensional Ising model, following a suggestion of Sykes (private communication) that the recurrence relation satisfied by the Onsager solution would be a worthy object of study.

In this method, the available series coefficients are used to define a linear differential equation with polynomial coefficients. The differential equation may be homogeneous or inhomogeneous. Details and examples of the method are given in a recent review [4].

In the intervening twenty years, a large number of models have been solved, many by Baxter and co-workers [5]. Many of these do not obviously satisfy the family of differential equations that underlie the D.A. method. Our initial analysis indicates that the underlying family of equations in most of these cases is an algebraic equation, of the form

$$\sum_{m=0}^{\mathrm{k}} P_m(x) f(x)^m = 0, \tag{1}$$

where the $P_m(x)$ are polynomials, and $f(x)$ is the solution of the model system. If the degree of the polynomial $P_m(x)$ is α_m, we denote the algebraic equation by $[\alpha_{\mathrm{k}}, \alpha_{\mathrm{k}-1}, ..., \alpha_1, \alpha_0]$. The properties of such algebraic equations are less well known than are the properties of the corresponding differential equation, in which the m'th power of $f(x)$ is replaced by the m'th derivative of $f(x)$. It is the latter differential equation that is satisfied by D.As.

We have developed a method of series analysis based on the above algebraic equation. The idea is the following: One has the first 10-100 terms of the power series expansion of $f(x)$. For each order of the algebraic equation, one systematically increases the degrees of the polynomials $P_m(x)$, demanding term by term agreement with the coefficients of the formal expansion of (1). It can be shown that this is sufficient for uniqueness up to a constant multiple. The situation is analogous to ordinary Padé approximants, to which indeed (1) reduces in the case k = 1. One then analyses the resulting algebraic equation in order to determine the critical points and critical exponents. The case k = 2 has also been discussed previously by Schafer [6], who called them quadratic Padé approximants.

The method is in some sense more restrictive than the D.A. method, as it can only yield rational critical exponents. For k = 1, only poles and zeros can be simulated. For k = 2, exponents involving half-integral powers can be obtained as well, with more complicated powers being obtained for higher values of k. However as most exactly solved models have rational exponents, this is less a restriction than a development of a method particularly appropriate to the study of such models.

With this method, we hope to provide a uniform classification of as many exactly solved models as possible, and, of perhaps greater significance, to search for solutions of previously unsolved models. The classification scheme proposed could include systems that are not classifiable within the framework of Conformal Field Theory, such as the chiral Potts model.

Those familiar with the theory of such algebraic equations will be aware that any such k^{th} order algebraic equation satisfies a homogeneous differential equation with polynomial coefficients of order k , or an inhomogeneous differential equation of the same type of order (k − 1). At first sight then it might appear that the proposed method offers no more than the existing differential approximant method. As a mathematical statement, this view is correct. As a method of series analysis however, this view is quite misleading for the following reason: In general we have only a finite number of series coefficients to work with. Thus we seek that representation of the solution that is the *most economical* in terms of the number of series coefficients needed for its specification. This is usually the algebraic equation representation. As an example we note that the magnetisation of the triangular lattice Ising model with pure triplet interactions [7] satisfies an algebraic equation of type $[1, 1, \phi, 0, 0]$, while the corresponding homogeneous differential equation is of type $[5, 4, 3, 2]$. (The notation used here is analogous to that used for the algebraic equations - the m'th entry refers to the degree of the polynomial multiplying the $(\mathrm{k}-m+1)^{th}$ derivative. The algebraic equation thus requires 5 series coefficients for its discovery, while 17 series coefficients are needed to find the corresponding differential equation. To show that this is generally (though not invariably) true, we note that Hunter and Baker [2] have shown that if a function $f(x)$ is the solution of a quadratic algebraic equation

$$Pf^2 + Qf + R = 0$$

where P, Q and R are polynomials in x, then $f(x)$ also satisfies the first-order inhomogeneous differential equation,

$$\begin{aligned}(PQ^2 - 4P^2R)f'(x) + (2P^2R' - PQQ' + P'Q^2 - 2PP'R)f(x) \\ + (P'QR - 2PQ'R + PQR') = 0.\end{aligned}$$

If P,Q and R are all of the same degree, n say, the polynomials multiplying the derivatives are of degree $3n$,$3n-1$ and $3n-1$ respectively (ignoring the possibility of factorizations or cancellations). Thus 3 times as many series coefficients are required to determine the differential equation representation from the series coefficients than are required to determine the algebraic equation representation. This result can be generalized. Let the algebraic equation (1) be written in the form

$$G(f, x) = 0, \tag{2}$$

which defines f implicitly as a function of x (or vice versa). The elimination of f between (2) and

$$\frac{\partial G}{\partial f} = 0$$

gives a polynomial, $D(x)$ called the discriminant. It can be shown [12] that the homogeneous differential equation satisfied by $f(x)$ is of the general form,

$$Q_m D^m \frac{d^m f}{dx^m} + \ldots + Q_2 D^2 \frac{d^2 f}{dx^2} + Q_1 D \frac{df}{dx} + Q_0 f = 0$$

where the Q_n are polynomials in x. It is clear that unless their are fortuitous cancellations, there is a large redundancy in the differential equation representation as successive powers of the *same* polynomial, that is $D(x)$, appear in each coefficient. A similar form holds for the inhomogeneous differential equation. The series coefficients used in fitting to a D.A are therefore wasted on the higher powers of the discriminant. As an example, the mean number density ρ, of the hard hexagon model [11] satisfies the algebraic equation

$$3(1-11z-z^2)\rho^4-(1-66z-11z^2)\rho^3-15z(3+z)\rho^2+3z(4+3z)\rho-z(1+2z) = 0$$

were z is the reciprocal activity. The polynomial coefficients of the corresponding differential equation are

$$\begin{aligned}
P_0(z) =& 40(-50 - 204z - 3462z^2 + 21999z^3 + 3462z^4 - 204z^5 + 50z^6),\\
P_1(z) =& 40(-68 + 926z + 9768z^2 - 52419z^3 - 149952z^4 + 32394z^5\\
&- 95291z^6 - 17954z^7 - 558z^8 + 11z^9),\\
P_2(z) =& 4R(z)(-30 + 2194z + 26526z^2 - 493774z^3 + 52405z^4 - 415340z^5\\
&- 271417z^6 - 16473z^7 + 352z^8),\\
P_3(z) =& 36zR(z)^2(6 + 6z - 3620z^2 + 1600z^3 - 6630z^4 - 1013z^5 + 22z^6),\\
P_4(z) =& 9z^2R(z)^3(-6 - 184z + 120z^2 - 504z^3 + 11z^4),
\end{aligned}$$

where $R(z) = -1 + 11z + z^2$. The algebraic equation is a [2,2,2,2,2] equation, requiring 14 coefficients, whilst the differential equation is a [12,11,10,9,6], equation requiring 52 coefficients.

Our method involves systematically fitting algebraic equations of specified order to existing series expansions of solved and unsolved problems. The algebraic equation in each case can be analysed to produce estimates of the critical parameters and predictions of subsequent series coefficients. In principle, this parallels work done previously in the development of the differential approximant method. However the theory of algebraic equations is less widely known than is the corresponding theory of ordinary differential equations. Accordingly, considerable work is still needed to find, or develop, suitably rapid algorithms for obtaining the discriminant of the multivariable polynomials that arise, and the subsequent analysis to predict the critical exponent. The possibility of introducing constraints corresponding to known critical points and exponents will also be considered.

As an example of classifying known solutions, our preliminary work has shown that the problem of convex polygons [8] satisfies a second order algebraic equation of size $[4, 7, 10]$. We have also solved the problem of row-convex polygons [9], which had not previously been solved, except implicitly [10]. The solution satisfies (1) with k = 4, and is given by a $[3, 4, 5, 6, 6]$ algebraic equation.

2 Method of Analysis

For an algebraic equation of the form (1), one must first decide on the order of the equation. All values of k > 1 could be chosen, but bearing in mind that this method is likely to be most useful in the situation where one has a rational exponent, the exponent may be known or conjectured. If it is believed that the exponent corresponds to a square root branch point, then a quadratic, or quartic, or quadratic in $f(x)^2$, is an appropriate algebraic equation. Similarly, an exponent of 1/9 dictates a 9th order algebraic equation, or a cubic in $f(x)^3$. Once the order is decided upon, our procedure is simply to increase the degree of the polynomials until one runs out of series coefficients. At each stage, the system of equations that must be solved to determine the polynomial coefficients is linear. If an exact algebraic equation is "discovered" by this process, the coefficients suddenly become integral or rational. Increasing the degrees of the polynomial beyond the minimum required to specify the exact solution does not change this observation. That is to say, once an exact representation is found, the approximant "locks in" to that representation, and higher degree polynomial coefficients are found to be zero (or numerically very small).

Of course the discovery of such an approximant does not constitute a rigorous derivation of the result, but if one obtains an algebraic equation that reproduces all known series coefficients (including many not used in the derivation of the approximation) and produces the exact critical point(s) and exponents (if known), the likelihood that the conjecture is wrong is infinitesimally small. Further, once the solution has been conjectured, it should be far easier to find the exact solution by traditional mathematical methods, as we were able to do for the row-convex polygon problem [9].

The next step is the analysis of the approximant in order to find the critical point and critical exponent. Consider (1) for some fixed numerical value of x. Then we just have a polynomial of order k with real coefficients which thus has in general k roots $f_1, f_2, \ldots, f_{\mathrm{k}}$. As x changes, each of the f_i change. Thus (1) gives rise to k functions of x, that is $f_i(x)$, $i = 1, 2, \ldots, \mathrm{k}$. These are the k elements or branches of $f(x)$. If for any given x, all the branches are distinct and finite, then x is a regular point, otherwise the point is called an exceptional point. Exceptional points may be either regular or singular. The exceptional points arise from three sources i) the roots of $P_{\mathrm{k}}(x) = 0$ which correspond to one or more of the the f_i being infinite (these are always singular points), ii) the roots of $D(x) = 0$ which are points where more than two branches of f have the same value (these are not necessarily singular points), and iii) the point at infinity may be singular.

The critical exponent is related to the cyclic structure of the branches in the neighbourhood of the critical point x_c. First consider an exceptional point derived from case ii). Without loss of generality the point can be shifted to the origin, so $x = 0$ is the exceptional point. Now, suppose n of the roots of

$$G(f, 0) = 0$$

are *equal*, where $1 < n \leq \mathrm{k}$. Let $f = 0$ be the value of the root (if $f \neq 0$ then shift it to the origin). Thus in the neighbourhood of $x = 0$ we have n roots $f_1(x), f_2(x), \ldots, f_n(x)$ which tend to zero as x tends to zero. These functions are defined on a punctured disc and are analytic in the neighbourhood of any point on the disc, but not necessarily single-valued. (The radius of the disc is made small enough so that $x = 0$ is the only singular point on the disc.)

Consider a circular path C in the disc, centered on the puncture $x = 0$. Consider $f_1(x)$ and move along C starting at some point on C, then upon returning to the starting point $f_1(x)$ may return to its original value or may equal another element $f_2(x)$, if upon repeating the cycle the value of $f_2(x)$ returns to the original value $f_1(x)$ then we have a two-cycle. It follows that $f_1(z^2)$ must be a single valued function of z and thus possess a power series expansion in z, that is

$$f_1(z) = \sum_{m=1}^{\infty} c_m z^m$$

which, for each solution of $z^2 = x$, gives an expansion of the form

$$f_1(x) = \sum_{m=1}^{\infty} c_m x^{m/2}.$$

Thus we have an expansion in *fractional* powers of x. This is an example of a Puiseux expansion. In the general case, κ of the branches may be permuted upon describing C κ times, giving rise to a κ-cycle. Similarly, $f_1(z^\kappa)$ is single valued and possesses a power series expansion in z which, in x, is of the form

$$f_1(x) = \sum_{m=1}^{\infty} c_m x^{m/\kappa}. \qquad (3)$$

for each solution of $z^\kappa = x$. The remaining $\mathrm{k} - n$ roots are considered in the same way. Thus we obtain a set of cycles $\{\kappa_1, \kappa_2, \ldots, \kappa_\mu\}$, with $\kappa_1 + \kappa_2 + \ldots + \kappa_\mu = \mathrm{k}$. If $\kappa_i = 1$ then the branch is regular and if $\kappa_i > 1$ the branches form an "algebriac element" of $f(x)$.

It is clear then that if $f(x)$ is some thermodynamic function which goes to zero at x_c (the physical singularity), then the Puiseux expansion gives

$$f_1(x) \sim c_{m_0}(x - x_s)^{m_0/\kappa} \qquad\qquad m_0 > 0$$

thus identifying m_0/κ as the critical exponent (m_0 is the first non-zero term in the Puiseux expansion). Thermodynamic functions which diverge as $x \to x_c$ arise from case i), the roots of $P_{\mathrm{k}}(x) = 0$. Let x_c be a root, and shift it to the origin. Thus $G(f, 0) = 0$ now has only $n <$ k roots. These are either algebraic or regular as discussed above. There remain the $\mathrm{k} - n$ roots that tend to infinity as $x \to 0$. These are analysed as follows: Let $g = 1/f$, and form

$$F(g, x) = g^{\mathrm{k}} G(1/g, x),$$

then $F(g, 0) = 0$ has $\mathrm{k} - n$ roots which tend to zero as $x \to 0$. These roots can then be analysed in the same way as those above, leading to a Puiseux expansion for $g(x)$. If the first non-zero term in the expansion of a κ-cycle of $g(x)$ is $c_{m_0} x^{m_0/\kappa}$, then as $g = 1/f$, the series for $g(x)$ may be inverted giving

$$f_1(x) = x^{-m_0/\kappa} \sum_{m=0}^{\infty} d_m x^{m/\kappa}, \qquad\qquad (d_0 \neq 0).$$

This gives an expansion for thermodynamic functions behaving like,

$$f_1(x) \sim d_{m_0}(x - x_s)^{-m_0/\kappa} \qquad\qquad (m_0 \neq 0)$$

and hence the critical exponent is $-m_0/\kappa$.

Thus to obtain the critical exponent it is necessary to obtain at least the first (non-zero) term in the Puiseux expansion. There exists a well defined algorithm for obtaining the Puiseux expansion which uses "Newton's diagram" [13]. The algorithm is well suited to programming. In this way each algebraic approximant may be analyzed. The Puiseux expansion can also be developed to arbitrary order, which can be used to predict coefficients of the original series expansion and so lead to a conjectured exact solution (as explained above).

In addition, if the cycle index of all the singular points can be determined, it is then possible to calculate the genus of the Riemann surface on which the algebraic function is single-valued. This is of interest as it tells us something about the type of automorphic functions which uniformize the algebraic function. These are the functions which arise naturally in exact solutions [5].

3 Discussion and Conclusion

We believe that the method of algebraic approximants is a potentially powerful series analysis tool for the study of systems believed to have rational critical exponents. Many two-dimensional systems exhibit this property, as do systems above their critical dimensionality. (Systems at their critical dimensionality usually have confluent logarithmic singularities, which in most cases therefore lie outside the framework of the algebraic approximants we have considered). A further development of these ideas is the generalization of (1) to a two (or more) variable version, of the form

$$\sum_{m=0}^{\mathrm{k}} P_m(x,y) f(x,y)^m = 0$$

which will then allow, in principle, for the study of multicritical points, and constitutes a particularisation of the PDA method for multivariable functions. In parallel with this numerical and theoretical work, we propose to study known exact solutions with a view to categorising them according to the underlying algebraic equation and to determine their genus.

4 References

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