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LETTER TO THE EDITOR

A special series expansion technique for the square lattice

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Abstract. The partition functions of generalised Ising-type models on the square lattice can be approximated in terms of the partition functions for finite $n \times n$, $n \times (n-1)$ and $(n-1) \times (n-1)$ lattices. When expressed as high-temperature series, these approximations give terms through to order $2n$ or $2n+1$ correctly.

Series expansion methods in statistical mechanics have recently shown a trend towards increasing algebraic complexity (see for example Sykes *et al* 1965, Wortis 1974, Sykes *et al* 1975). A closer examination of these techniques shows that this increase in algebraic complexity is a result of reducing the combinatorial complexity. De Neef and Enting (1977) have discussed a number of the reasons why such a trade-off between algebraic complexity and combinatorial complexity should be desirable in practical computations.

The method introduced by de Neef (1975) for series expansions of square lattice models represents an extreme example of the trend away from combinatorial complexity since series to order $4n-2$ can be obtained by considering only $n(n-1)$ graphs in contrast to the exponential growth in the number of graphs required by most other techniques. The graphs used by de Neef were $\{G_{mk};\ m+k \leq 2n+1\}$, the G_{mk} being strong (or section) subgraphs of the square lattice defined by $m \times k$ rectangular arrays of vertices.

We wish to point out that the reduction of graphs can be taken one stage further and that expansions on the square lattice, correct to order $2n$, can be obtained by considering only G_{nn}, G_{mn}, G_{mm}, $m = n-1$. If we let $Z(G_{mk})$ denote the partition function for a particular system defined on graph G_{mk} and let $\bar{Z}$ denote the limit as $r \to \infty$ of $Z(G_r)^{1/r^2}$ then approximations for $\bar{Z}$ are given by

$$\bar{Z} \approx Z(G_{nn})Z(G_{mm})/Z(G_{mn})Z(G_{nm}) \qquad m = n-1. \tag{1}$$

Only when the model has a lattice anisotropy is it necessary to consider G_{mn}, G_{nm} separately.

The origins of the idea of using (1) as a useful approximation for Z lie in two distinct (though related) sources. One approach comes from the work of Baxter (1968). This leads to a variational expression for $\bar{Z}$ (equation (3.12) of Baxter 1968 where $\bar{Z}$ is denoted as κ). A simple choice of trial functions in this expression leads to equation (1) above.

The other approach that leads to expression (1) is the work of Hijmans and de Boer (1955) which gives a systematic treatment of the cluster-variation approximation of

Kikuchi (1951). Hijmans and de Boer considered a cluster sum involving G_{nn} and all its subgraphs. They then showed that the only subgraphs that contributed to the sum were G_{jk}, j, $k \leq n$. In fact it is shown below that only G_{nn}, G_{mn}, G_{nm}, G_{mm}, $m = n-1$ contribute. Hijmans and de Boer investigated the $n = 3$ case and noted that only G_{33}, G_{32} and G_{22} contributed but failed to notice the reduction for general n. The relations that show the reduction are purely combinatorial and so the reduction does not depend on whether one considers a system with effective fields (as in the Kikuchi approximation) or simply a truncated lattice (as in finite-cluster sums used for series expansions).

The derivation starts by considering models for which a finite-cluster expansion, in terms of closed graphs (no order 1 vertices), exists for the 'free energy' f_α of any graph α:

$$f_\alpha = \ln(Z(\alpha)) = \sum_{\beta \subseteq \alpha} c_{\alpha\beta} h_\beta \tag{2}$$

where $\subseteq$ denotes the subgraph relation and $c_{\alpha\beta}$ is the number of ways β occurs as a subgraph of α, and h_β is of order $e(\beta)$, the number of edges of β, in an appropriate expansion variable. The graphs considered are 'labelled' or 'oriented' so that edges are along different lattice directions (x or y) are regarded as different types of edges. This distinction is essential for anisotropic lattices and using this convention in defining $c_{\alpha\beta}$ simplifies the combinatorial arguments used in transforming equation (5). Either by recursive definition or by inverting a truncation of matrix $\mathbf{c}$, the h_β can be expressed in terms of the f_α by

$$h_\beta = \sum_{\alpha \subseteq \beta} d_{\beta\alpha} f_\alpha. \tag{3}$$

Formally we have

$$f = \ln Z = \sum_\beta h_\beta \tag{4}$$

and we consider the approximation

$$f \approx f^{(n)} = \sum_{\beta \subseteq G_{nn}} h_\beta \tag{5a}$$

$$= \sum_{\beta \subseteq G_{nn}} [(n - r_\beta + 1)(n - p_\beta + 1) - (n - r_\beta)(n - p_\beta + 1) - (n - r_\beta + 1)(n - p_\beta) + (n - r_\beta)(n - p_\beta)] h_\beta. \tag{5b}$$

If we let r_β, p_β be the r, p of the smallest G_{rp} of which the (oriented) graph β is a subgraph then expression (5) corresponds to

$$f \approx f^{(n)} = \sum_{\beta \subseteq G_{nn}} (c_{G_{nn},\beta} + c_{G_{mm},\beta} - c_{G_{mn},\beta} - c_{G_{nm},\beta}) h_\beta, \qquad m = n - 1. \tag{6}$$

Using (2) and taking the exponential of (6) gives

$$Z \approx Z(G_{nn}) Z(G_{mm}) / Z(G_{mn}) Z(G_{nm}). \tag{7}$$

These combinatorial arguments make the generalisation to higher dimension obvious.

The models for which (7) can be used to give series expansions are those for which a finite-cluster sum of the form of (2) exists. These models include the Ising model in zero field, the Potts models in zero field and by extension from the Potts models, the

technique applies for series expansions of the infinite lattice limit of chromatic polynomials (see Enting 1977).

The number of series terms depends on the approximation (5*a*). If the Ising or Potts models are expanded in terms of $\beta = 1/kT$ then the first incorrect term is β^{2n} so that the Potts model is correct to β^{2n-1} in general or β^{2n-2} in the Ising case where only even powers of β occur. The first missing graph is the $1\times(n+1)$ rectangle. If however the functions $f_\alpha - e(\alpha)\ln\lambda_0$ are expanded in powers of λ_1/λ_0 (see Domb 1974 for definitions) then the $1\times(n+1)$ graph does not contribute, the smallest missing graph is $2\times(n+1)$ and the first incorrect coefficient is that of $(\lambda_1/\lambda_0)^{2n+2}$. The general Potts model is correct to order $2n+1$ and the Ising model case where $\lambda_1/\lambda_0 = \tanh\beta J$ is correct to order $2n$. The limit of chromatic polynomials is given as

$$W(q) = q^{-1}(q-1)^2\left(1+\sum a_k(q-1)^{-k}\right) \tag{8}$$

with a_k given correctly through to a_{2n}.

We conclude our discussion by comparing the method described above to the technique of de Neef (1975). This latter technique is obtained from the same combinatorial properties described by Hijmans and de Boer (1955) but replaces the maximal graph G_{nn} by a maximal set $G_{k,n-k}$. If the $Z(G_{jk})$ are constructed using direct transfer matrix techniques, $Z(G_{jk})\rightarrow Z(G_{j,k+1})$ then for a given size of transfer matrix, the de Neef technique gives almost twice as many terms as can be obtained from (7) with little extra computation.

There is however an alternative procedure for calculating the $Z(G_{nn})$ and that is to use the corner-transfer-matrices described by Baxter (1976). This procedure can be adapted to calculating the 'nearly-square' case $Z(G_{nm})$ but is not suitable for general G_{mk}. The existence of the corner-transfer-matrix method which uses smaller matrices than the direct row by row transfer matrix, makes expansions based on (7) comparable with the de Neef technique in the amount of computation required.

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