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Generalised Möbius functions for rectangles on the square lattice

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Abstract. Finite cluster expansions are described in terms of generalised Möbius functions. This description is used to formalise techniques for obtaining series expansions for lattice models in terms of rectangular graphs. In particular new expressions are given for boundary corrections for finite systems.

1. Introduction

Within the last two years there have been several papers showing how to obtain series expansions for lattice statistics problems defined on infinite square lattices in terms of rectangular subgraphs of the square lattice. De Neef (1975) applied one such method to obtaining series expansions for the Potts model. This approach was formalised by de Neef and Enting (1977). Enting and Baxter (1977) described a related expansion technique which was suggested by variational approximations used by Baxter (1968) and which turned out to be based on combinatorial relations equivalent to those used by Hijmans and de Boer (1955) for closed form approximations. Enting (1977) has investigated these rectangular graph expansions from the point of view of computational efficiency and shown that is some cases the rectangular graph expansions can be proved to be more efficient than conventional expansion techniques. Kim and Enting (1978) have applied the de Neef formalism to deriving series expansions for the infinite limit of chromatic polynomials.

The present paper uses a generalisation of Möbius functions (Rota 1964, Wilson 1971) to demonstrate the unity of the combinatorial results underlying the two methods of Enting and Baxter, and de Neef. A number of new results are presented including explicit general inverses for the T matrices $c_{\alpha\beta}$ used by de Neef and Enting (1977) and thence explicit general expressions for the expansion coefficients. In addition it is shown that the rectangular lattice expansions can be used to obtain expressions for the boundary contributions for finite systems. These boundary contributions are of interest in physical problems because of effects such as grain size in crystals and the possibility of directly observing surface effects (Watson 1972). Boundary effects in the Ising model and related models are also of interest to statisticians since the Ising model is equivalent to a Markov random-field defined on binary variables (see for example Besag 1974, Pickard 1976). Since the boundary corrections to correlation functions will always be of the same order of magnitude as the confidence intervals associated with finite size sampling errors, (Martin-Löf 1973, Pickard 1977) such confidence intervals will be meaningless unless expressions for boundary contributions can be obtained.

In § 2 the Möbius functions used in combinatorial analysis are generalised in a manner appropriate to series expansion techniques. This generalisation is applied to rectangular graph expansions in § 3 and the appropriate Möbius functions are given. In § 4 these generalised Möbius functions are summed to give expressions for series expansions for both the de Neef and the Enting and Baxter formalisms and in a form which explicitly gives boundary corrections.

2. Generalisations of Möbius functions for series expansions

In combinatorial analysis, Möbius functions are defined as elements of incidence algebras over partially ordered sets, X (Rota 1964, Wilson 1971). In the series expansion formalisms the sets involved will be sets of graphs with the subgraph relation as the ordering relation. Multiplication in an incidence algebra is defined as an inner product:

$$f(x, y) = \sum_{z\in X} g(x, z)h(z, y). \tag{2.1}$$

If one defines the incidence function $\zeta(x, y)$ by

$$\zeta(x, y) = \begin{cases} 1 & x \leqslant y \\ 0 & \text{otherwise} \end{cases}$$

then its inverse, $\mu(x, y)$ is defined so that

$$\sum_{y} \mu(x, y)\zeta(y, z) = \begin{cases} 1 & x = z \\ 0 & \text{otherwise.} \end{cases} \tag{2.2}$$

The Möbius function $\mu(x, y)$ can be used to transform sums over sets so that if

$$f(x) = \sum_{y\leqslant x} h(y)$$

then

$$h(x) = \sum_{y\leqslant x} f(y)\mu(y, x). \tag{2.3}$$

The application series expansions arise if $f(y)$ is a function such as the free energy of a particular model defined on graph g and which can be expressed as

$$f(g) = \sum_{g'\leqslant g} h(g')$$

and which for large graphs G can be usefully approximated by

$$f(G) \approx \sum_{g'\leqslant g''} h(g').$$

Then $f(G)$ can be expressed, approximately, in terms of the $f(g)$, $g \leqslant g''$. This formalism is essentially that of Domb (1974) and it requires that the set of graphs be labelled so that any graph occurs at most once as a subgraph of a given graph.

In terms of unlabelled graphs,

$$f(g) = \sum_{g'} h(g')t(g', g) \tag{2.4}$$

where $t(g', g)$ is the number of ways that g' occurs as a subgraph of g, and thus corresponds to the T matrix used in lattice statistics and is a generalisation of the incidence function $\zeta(x, y)$. The inverse of t, $\nu(g, g')$ can thus be regarded as a generalisation of the Möbius function, and we write:

$$f(G) \approx \sum_{g, g' \leqslant g''} f(g)\nu(g, g')t(g', G). \tag{2.5}$$

These equations can be generalised by replacing g'' by a set Γ of cutoff graphs so that all the sums are over those graphs which are subgraphs of at least one graph in Γ. A typical set Γ would be the set of all graphs of m lines, in many models, would lead to an approximation of the form (2.5) which was correct to order m in an appropriate expansion variable.

3. Generalised Möbius functions for rectangles

To apply the formalism of the preceding section we have to select a function f and find a set of graphs for which the h functions lead to a useful approximation. A typical application is to have f as the free energy for some lattice model such as the Potts model and to have g as the set of connected subgraphs of some infinite lattice L which is defined as the limit of a sequence of finite lattices L_n. The equations of the previous section become

$$\begin{aligned} f &= \lim_{n\to\infty} f(L_n) \\ &= \lim_{n\to\infty} \sum_{g'} h(g')t(g', L_n) \\ &\approx \sum_{g' \leqslant \Gamma} h(g') \lim_{n\to\infty} t(g', L_n) \\ &= \sum_{g, g' \leqslant \Gamma} f(g)\nu(g, g') \lim_{n\to\infty} t(g', L_n). \end{aligned} \tag{3.1}$$

It has been shown (Hijmans and de Boer 1955, de Neef 1975 and de Neef and Enting 1977) that if L is the square lattice and if a function f has an expansion in terms of the $f(g)$ where the graphs g are all connected, then f has an expansion in terms of the $f(r)$ where the graph r is a rectangle. The rectangular graphs are denoted $[m, n]$ and correspond to the set of $n \times m$ vertices indexed $\langle i, j\rangle$, $1 \leqslant i \leqslant m$, $i \leqslant j \leqslant n$ with edges connecting $\langle i, j\rangle$ to $\langle i+1, j\rangle$ and $\langle i, j+1\rangle$.

For these rectangular graphs, the T matrix is

$$t([i, j], [m, n]) = \begin{cases} (m-i+1)(n-j+1) & \text{if } i \leqslant m \text{ and } j \leqslant n \\ 0 & \text{otherwise.} \end{cases} \tag{3.2}$$

The inverse of this T matrix is given by the generalised Möbius function

$$\nu([i, j], [m, n]) = \eta(i, m)\eta(j, n) \tag{3.3}$$

where

$$\eta(i, m) = \begin{cases} 1 & \text{if } i = m \text{ or if } i+2 = m \text{ and } m > 2 \\ -2 & \text{if } i+1 = m \text{ and } m > 1 \\ 0 & \text{otherwise.} \end{cases} \tag{3.4}$$

This result is easily verified by taking the product of the ν and t functions. Equations (3.4) gives

$$h([i,j])=f([i,j])-2f([i,j-1])+f([i,j-2])-2f([i-1,j])+4f([i-1,j-1])$$
$$-2f([i-1,j-2])+f([i-2,j])-2f([i-2,j-1])+f([i-2,j-2]). \quad (3.5)$$

4. Applications

To obtain series expansions for boundary effects, consider the expansions for the graph $[M, N]$ which take the form

$$f([M,N])\approx\sum_{[i,j],[m,n]\leqslant\Gamma} f([i,j])\nu([i,j],[m,n])t([m,n],[M,N]). \quad (4.1)$$

The non-zero elements of the T matrix take the values

$$(M-m+1)(N-n+1)=MN-N(m-1)-M(n-1)+(m-1)(n-1) \quad (4.2)$$

so $f([M, N])$ will have a 'bulk' contribution from the MN term, 'edge' contributions from the $N(m-1)$ and $M(n-1)$ terms and a 'corner' contribution from the remaining terms.

There are two choices for the cutoff set Γ which we consider: $A(k)$ the set used by Enting and Baxter (1977) and $B(k)$ the set used by de Neef (1975).

$$A(k)=\{[k,k]\} \quad (4.3)$$

$$B(k)=\{[i,j]: i+j=k\}. \quad (4.4)$$

There are two basic sums over the $\eta(i,n)$ which we have to consider when using set $A(k)$:

$$\sum_{n=1}^{k}\eta(i,n)=\delta_{i,k}-\delta_{i,k-1} \quad (4.5)$$

$$\sum_{n=1}^{k}n\eta(i,n)=k\delta_{i,k}-(k+1)\delta_{i,k-1}. \quad (4.6)$$

Substituting these sums into (4.1) with cutoff set $A(k)$, the contribution of $f([i,j])$ to $f([M,N])$ is given by

$$MN(\delta_{ik}-\delta_{i,k-1})(\delta_{jk}-\delta_{j,k-1})-M((k-1)\delta_{ik}-k\delta_{i,k-1})(\delta_{jk}-\delta_{j,k-1})$$
$$-N(\delta_{ik}-\delta_{i,k-1})((k-1)\delta_{jk}-k\delta_{jk})+((k-1)\delta_{ik}-k\delta_{i,k-1})$$
$$\times((k-1)\delta_{jk}-k\delta_{j,k-1}). \quad (4.7)$$

As long as the system is isotropic so that $f([i,j])=f([j,i])$ the factors that multiply M and N will be equivalent so that there will be an edge contribution which for any M, N is proportional to $(M+N)$. Of course all of the discussion above assumes $M\geqslant k$, $N\geqslant k$. For small values of M or N $f([M,N])$ can be calculated directly using the transfer matrices used to obtain the $f([i,j])$ and so series expansions for $f([M,N])$ are irrelevant. The bulk contribution in (4.7) reproduces the expression given by Enting and Baxter (1977) but the other expressions are apparently new.

When the cutoff set $B(k)$ is used, the sums over the η functions cannot be performed independently. We have to consider the sums

$$\begin{aligned}\sum_{m=1}^{k-1}\sum_{n=1}^{k-m}\eta(i,m)\eta(j,n)\\&=\sum_{m=1}^{k-1}\eta(i,m)(\delta_{j,k-m}-\delta_{j,k-m-1})\\&=\eta(i,k-j)-\eta(i,k-j-1)\\&=\delta_{i,k-j}-3\delta_{i,k-j-1}+3\delta_{i,k-j-2}-\delta_{i,k-j-3}\end{aligned}\tag{4.8}$$

$$\begin{aligned}\sum_{m=1}^{k-1}\sum_{n=1}^{k-m}m\eta(i,m)\eta(j,n)\\&=(k-j)\eta(i,k-j)-(k-j-1)\eta(i,k-j-1)\\&=(k-j)\delta_{i,k-j}-(3k-3j-1)\delta_{i,k-j-1}+(3k-3j-2)\delta_{i,k-j-2}\\&\quad-(k-j-1)\delta_{i,k-j-3}\end{aligned}\tag{4.9}$$

$$\begin{aligned}\sum_{m=1}^{k-1}\sum_{n=1}^{k-m}mn\eta(i,m)\eta(j,n)\\&=\sum_{m=1}^{k-1}m\eta(i,m)[(k-m)\delta_{j,k-m}-(k-m+1)\delta_{j,k-m-1}]\\&=j(k-j)\eta(i,k-j)-(k-j-1)(j+2)\eta(i,k-j-1)\\&=ij\delta_{i,k-j}-(3ij+2i+2j)\delta_{i,k-j-1}+(3ij+4i+4j+4)\delta_{i,k-j-2}\\&\quad-(j+2)(i+2)\delta_{i,k-j-3}.\end{aligned}\tag{4.10}$$

Substituting these sums into (4.1) with $B(k)$ used as the cutoff set G shows that the contribution of $f([i,j])$ to $f([M,N])$ is given by

$$\begin{aligned}MN(\delta_{i,k-j}-3\delta_{i,k-j-1}+3\delta_{i,k-j-2}-\delta_{i,k-j-3})\\&+N((1-i)\delta_{i,k-j}+(3i-1)\delta_{i,k-j-1}-(3i+1)\delta_{i,k-j-2}+(i+1)\delta_{i,k-j-3})\\&+M((1-j)\delta_{i,k-j}+(3j-1)\delta_{i,k-j-1}-(3j+1)\delta_{i,k-j-2}+(j+1)\delta_{i,k-j-3})\\&+(i-1)(j-1)\delta_{i,k-j}+(1+i+j-3ij)\delta_{i,k-j-1}+(3ij+i+j-1)\delta_{i,k-j-1}\\&-(i+1)(j+1)\delta_{i,k-j-3}.\end{aligned}\tag{4.11}$$

The 'bulk' term had been obtained in particular cases by de Neef (1975), de Neef and Enting (1977) and Kim and Enting (1978). The general solution had not been noticed because the contributions of $f([i,j])$ and $f([j,i])$ were combined when possible. Again the expressions for boundary effects are apparently new.

5. Conclusions

The expansions in the previous section have demonstrated the common combinatorial results which connect the expansion technique of de Neef (1975) to that of Enting and Baxter (1977). In addition the formalisms have been generalised to show how boundary terms can be expressed in terms of the same functions which are used to calculate bulk contributions. The fact that these expressions include the corner corrections should make them useful for the statistical analysis of spatial data when comparatively small-sized regions are being investigated. The physical significance of boundary effects has been reviewed by Watson (1972) but most of the emphasis has been on fairly large systems for which boundary effects are significant only in the critical region.

In conclusion, it should be noted that in actual applications of the techniques described above, it will usually be more convenient to take the exponentials of the expressions given above so that the sums become products. In many cases such as the Ising and Potts models only integers will be involved in the calculations if product expressions are used. Rounding errors associated with the usual 'floating point' representation of real numbers in digital computers can thus be avoided without the difficulty of having to work with non-standard representations of rational numbers. This property has previously been noticed in algebraic graph theory calculations (Biggs 1974, Kim and Enting 1978) but seem to have been used very little, if at all, in theoretical physics.

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