1 · Resonance and reconstruction

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SUMMARY

This article is another attempt to reconcile part of graph theory and part of theoretical physics. Specifically, we shall discuss some aspects of the reconstruction problem in terms of simple models of physical phenomena. A previous essay in the same vein (Biggs 1977a, henceforth referred to as IM) may be consulted for background information and proofs of some basic theorems.

There are four sections: (1) Interaction Models, (2) the Algebra of Graph Types, (3) Reconstruction, (4) Partition Functions for Infinite Graphs.

1. INTERACTION MODELS

1.1 Definitions

Let G be a finite (simple) graph, with vertex set V and edge-set E. An 'interaction model' on G arises when the vertices of G may have certain attributes, and they interact along the edges according to the values of those attributes. To be more precise, let A denote a finite set of objects (attributes), and define a *state* on G to be a function $\omega: V \to A$. In graph theory, we often think of the attributes as colours, so that a state is a colouring. In theoretical physics, the vertices represent particles of some kind, and the attributes represent some physical property, such as a magnetic moment.

The interaction between a pair of adjacent vertices is measured by a real-valued function i, called the *interaction*

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function, defined on the set $A^{(2)}$ of unordered pairs of attributes. That is, $i\{a_1,a_2\}$ measures the interaction between a pair of vertices when they are joined by an edge and they have attributes a_1 and a_2. An *interaction model* M is a pair (A,i), where A is a finite set and i is an interaction function. Thus different interaction models may represent different physical contexts, while graphs represent possible geometrical configurations of particles to which the physical laws apply.

Suppose that an interaction model M and a graph G are given. The total 'weight' $I(\omega)$ of a state ω on G is defined to be

$$I(\omega) = \prod_{\{u,v\}\in E} i\{\omega(u),\omega(v)\} .$$

(The reason for taking a product, rather than a sum, will be explained shortly.) The *partition function* for the model M on G is

$$Z(M,G) = \sum_{\omega:V\to A} I(\omega) . \qquad (1.1.1)$$

1.2 Examples

In models of physical phenomena, the weight $I(\omega)$ is usually represented by an expression of the form $\exp[H(\omega)/kT]$, where k is an absolute constant, T is the temperature, and $H(\omega)$ is a measure of the energy of the state ω. Thus every state has a positive weight, and $I(\omega)/Z$ represents the probability of finding the system in a state ω. The expression for $H(\omega)$ will be a sum of terms $X(e)$, one for each 'local interaction' (edge) of the system; thus

$$I(\omega) = \exp \frac{1}{kT} \sum_{e\in E} X(e) = \prod_{e\in E} \exp X(e)/kT .$$

So we have recovered the general formulation for $I(\omega)$, and justified the occurrence of the product. In general, we think of the partition function Z as the representative of the global properties of the system.

A specific example is the famous Ising model of magnetism. In this case, the vertices of the graph represent particles in a ferromagnetic substance, and the attributes are the two possible orientations of a magnetic moment, conventionally described as 'up' and 'down'. If two adjacent particles have the same orientation, they contribute an amount of energy $+L$ to $H(\omega)$, otherwise they contribute $-L$. In order to express this model in our general framework, we may replace 'up' and 'down' by 0 and 1, and define an interaction function for $A = \{0,1\}$ by

$$i\{0,0\} = i\{1,1\} = \varepsilon \quad , \qquad i\{0,1\} = \varepsilon^{-1} \quad ,$$

where $\varepsilon = \exp(L/kT)$. We shall denote this interaction model (A,i) by I_T and refer to it as the *Ising model at temperature* T.

An example more familiar to graph theorists is the *colouring model* C_u. Here A is a finite set of u $(= |A|)$ colours, and the interaction function is defined as follows:

$$i\{a_1,a_2\} = \begin{cases} 0 & \text{if } a_1 = a_2 \ , \\ 1 & \text{otherwise} \ . \end{cases}$$

In this model, the weight of a 'colouring' $\omega: V \to A$ of the vertices of a graph G is zero if any pair of adjacent vertices have the same colour, and 1 otherwise. Hence $Z(C_u,G)$ is simply the number of proper colourings of G when u colours are available.

1.3 Resonant Models

Both the Ising model I_T and the colouring model C_u have

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the property that the interaction function takes only two values: $i\{a_1,a_2\}$ has one value i_0 if $a_1 = a_2$, and another value i_1 in all other cases. We may think of such a model as representing a situation where two particles interact in a special way if they have the same attributes, and in some other (constant) way if not. This is a kind of resonance, and we shall refer to such an interaction model as a *resonant* model.

The definition (1.1.1) of the partition function shows that, if R is a resonant model, $Z(R,G)$ is essentially dependent only on the ratio i_0/i_1. For this reason, we shall confine our attention to a normalized resonant model R_β whose interaction function is given by

$$i\{a_1,a_2\} = \begin{cases} \beta & \text{if } a_1 = a_2 , \\ 1 & \text{otherwise} . \end{cases} \qquad (1.3.1)$$

The following result is perhaps the most important property of resonant models.

Theorem A Let $R_\beta = (A,i)$ be a resonant model with $|A| = u$ and interaction function i as in (1.3.1), and let $G = (V,E)$ be a graph. Then

$$Z(R_\beta,G) = u^{|V|} \sum_F (\beta-1)^{|F|} u^{-r(F)} \qquad (1.3.2)$$

The sum is taken over all subsets F of E, and $r(F)$ denotes the rank of the edge-subgraph $\langle F\rangle$.

Proof [IM, p.23].

Since $r(F) < |V|$ for all subsets F of E, Theorem A tells us that the partition function of a resonant model is a polynomial function of the number of attributes, u. In the case $\beta = 0$ we obtain the well-known chromatic polynomial,

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$Z(C_u,G)$. The significance of the polynomial property in the general theory will appear in Section 3.

It may be noted that the polynomial property, and the resonance property, are both related to the existence of a 'deletion and contraction' algorithm: see Vout (1978).

2. THE ALGEBRA OF GRAPH TYPES

2.1 Star Types and Graph Types

A *star type* is an isomorphism class of finite, simple, non-separable graphs. We shall use the symbol St to denote the set of star types. It is often convenient to use a pictographic representation for the smaller star types: St = {|,△,□,⧄,...} .

A *graph type* is a function t defined on St and taking non-negative integer values, only a finite number of which are non-zero. We shall use the symbol Gr to denote the set of graph types. A finite graph G has *type* t if, for each $\sigma \in$ St , G has $t(\sigma)$ blocks of star type σ . Thus two graphs of the same type are not necessarily isomorphic; however, we shall see that the equivalence relation 'of the same type' is the appropriate one for the study of interaction models.

We shall denote the vector spaces of complex-valued functions defined on St , and on Gr , by $\underset{\sim}{X}$ and $\underset{\sim}{Y}$ respectively. Since St may be regarded as a subset of Gr in the obvious way, we have a projection $J: \underset{\sim}{Y} \to \underset{\sim}{X}$ defined by $(Jy)(\sigma) = y(\sigma)$ $(\sigma \in \text{St})$.

2.2 Type-Invariants

A function f defined on the set of finite graphs is a *type-invariant* if $f(G_1) = f(G_2)$ whenever G_1 and G_2 have the same type. In order that f may be a type-invariant, it is clearly sufficient that it should be an isomorphism invariant (so that it is invariant for star types), and that it should be multiplicative over blocks:

$$f(G) = \Pi f(B) \quad ,$$

where the product is taken over the set of blocks B of G.

The partition function of an interaction model is not quite a type-invariant, since the multiplicative property does not hold. (The partition function for two disjoint blocks is not the same as that for two blocks with one common vertex.) However, it is easy to see how to remedy this difficulty. We define the *reduced* partition function of the model $M = (A,i)$. with $|A| = u$, to be

$$\bar{Z}(M,G) = Z(M,G)/u^{|V|} \quad .$$

Theorem B The reduced partition function $\bar{Z}(M,G)$ is a type-invariant.

Proof [IM, p.63].

Associated with any type-invariant function f there is a vector ϕ in $\underset{\sim}{Y}$ defined by $\phi(t) = f(T)$, where T is any graph of type t. Thus we may think of the reduced partition function, with respect to a given model, as an element of $\underset{\sim}{Y}$.

2.3 Counting Subgraphs

If s and t are graph types, we define c_{st} to be the number of edge-subgraphs of a graph S of type s which have type t. There are two ways of fitting these numbers into our algebraic framework. First, we may think of the array (c_{st}) as a matrix, so that we have a linear transformation $C: \underset{\sim}{Y} \to \underset{\sim}{Y}$, defined as follows:

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$$(Cy)(s) = \sum_t c_{st}\, y(t) \quad . \tag{2.3.1}$$

It is clear that, for each given s, the sum on the right-hand side involves only a finite number of non-zero terms c_{st}. Furthermore:

Theorem C The linear transformation C is invertible.

Proof We have only to notice that if the graph types are ordered in a suitable way (for instance, compatibly with increasing number of edges) then the matrix (c_{st}) is lower triangular, and its diagonal terms are non-zero. Hence the terms of an inverse matrix may be computed recursively in the usual way.

Another useful way of handling the numbers c_{st} is to define, for each graph type s, a vector c_s in $\underset{\sim}{Y}$ as follows:

$$c_s(t) = c_{st} \quad . \tag{2.3.2}$$

The vector c_s, giving the census of subgraphs of s, may be considered as the representative of a 'real' graph type s. The result of Theorem C implies that the vectors $\{c_s\}$ $(s \in Gr)$ form a basis for $\underset{\sim}{Y}$, so that each y in $\underset{\sim}{Y}$ may be expressed (uniquely) as a linear combination of the basis $\{c_s\}$. Thus y is a 'generalized' graph type.

The point of view developed in the previous paragraph was introduced by Whitney in his pioneering work on graph colouring. He noticed that c_s is determined by its projection Jc_s in $\underset{\sim}{X}$; more precisely:

Theorem D There is a (non-linear) operator $W: \underset{\sim}{X} \to \underset{\sim}{Y}$, independent of the graph type s, such that

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$$W(Jc_s) = c_s \quad (\text{for all} \quad s \in Gr) \quad .$$

Proof [IM, p.67]. (The first proof (Whitney, 1932) was rather complicated; he failed to invert a matrix. Fortunately, I had the help of Colin Vout, who did.)

2.4 Expansions in Algebraic Form

The polynomial expansion (1.3.2) for the partition function of a resonant model may be written in algebraic form. For convenience we introduce a new variable $z = 1/u$, where $u = |A|$ is the number of attributes, and use the reduced partition function. The formula (1.3.2) becomes:

$$\bar{Z}(R_\beta, G) = \sum_{F \subseteq E} (\beta-1)^{|F|} z^{r(F)} \quad . \tag{2.4.1}$$

The reduced partition function and the individual summands on the right-hand side are type-invariants. Thus, if we write $e(s)$ and $r(s)$ for the number of edges and the rank of a graph of type s, we may define vectors ρ_z and m_z in $\underset{\sim}{Y}$ as follows:

$$\rho_z(s) = \bar{Z}(R_\beta, S) \quad , \quad m_z(s) = (\beta-1)^{e(s)} z^{r(s)} \quad ,$$

where S is any graph of type s. If we now collect the terms in (2.4.1) according to the type of the subgraph $\langle F \rangle$, we obtain

$$\rho_z(s) = \sum_t c_{st} m_z(t) \quad .$$

Equivalently, $\rho_z = Cm_z$. In fact, this expression is quite general, and does not depend on the resonance property of the model. If ξ is the vector representing the reduced partition function of an interaction model M, then the invertibility of the transformation C ensures that there is a vector m in Y such that $\xi = Cm$. That is,

$$\xi(s) = \sum_t c_{st}\, m(t) \quad . \qquad (2.4.2)$$

It is helpful to interpret (2.4.2) in the following way: each subgraph of type t contributes an amount m(t) to the value of $\xi(s)$. In the case of a resonant model, we have the useful feature that the contributions are simple monomial expressions in β and u .

3. RECONSTRUCTION

3.1 The Reconstruction Problem

In this section we shall explain the relationship between the foregoing ideas and the 'reconstruction problem' in graph theory. The basic theory was first published by Tutte (1967); there is also an account of it in Biggs (1974). However, it was not until Tutte's more recent work became available that its relevance was generally recognised (Tutte, 1979).

Let G be a finite simple graph with vertex-set $V = \{v_1, \ldots, v_n\}$, and let G_i denote the vertex-subgraph $\langle V - v_i \rangle$ of G . (G_i is obtained from G by deleting v_i and the edges incident with it.) In the *vertex-reconstruction problem* we are given the set of graphs $\{G_1, \ldots, G_n\}$, unlabelled and unordered, and we ask how much information about G may be deduced: such information is said to be *reconstructible*. It is possible that G itself may be reconstructible, but in general this seems to be a difficult question. We shall show that the partition function $Z(\mathcal{R}, G)$ is reconstructible, for any resonant model $\mathcal{R}$.

We begin by taking a census of the non-separable vertex-subgraphs of G . For a given graph S of type s , and a given star type τ , define $k_{s\tau}$ to be the number of vertex-subgraphs of S which have type τ . Now each non-separable vertex-subgraph <W> of G is a vertex-subgraph of those G_i for which v_i is not in W. Thus if g denotes the type of G, and $\mathcal{H}$ denotes the family of types of $G_1, \ldots, G_n$, we have

$$\{|V| - v(\tau)\}k_{g\tau} = \sum_{h \in \mathcal{H}} k_{h\tau} , \tag{3.1.1}$$

where $v(\tau)$ is the number of vertices of the star type τ. From this, we deduce the following useful result.

<u>Theorem E</u> Suppose that σ and τ are two star types which occur as vertex-subgraphs of a graph G. The the number $k_{\sigma\tau}$ is reconstructible.

<u>Proof</u> Clearly, there is nothing to prove unless σ is the type of G. In that case, $k_{\sigma\sigma}$ is unity, and the other values of $k_{\sigma\tau}$ are determined by (3.1.1).

For example, let G be a graph of type ⧄. Then $\mathcal{H} = \{||, ||, \Delta, \Delta\}$ and we have

$$(4-2)k_{\text{⧄},|} = 2 + 2 + 3 + 3 ,$$

and so forth. The full set of relevant values of $k_{\sigma\tau}$ may be tabulated as follows:

	|	Δ	⧄
|	1	0	0
Δ	3	1	0
⧄	5	2	1

(3.1.2)