Characterizing partition functions of the spin model by rank growth

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Abstract. We characterize which graph invariants are partition functions of a spin model over $\mathbb{C}$, in terms of the rank growth of associated 'connection matrices'.

1. Introduction

In this paper, all graphs are undirected and finite and may have loops and multiple edges. An edge connecting vertices u and v is denoted by uv. Let $\mathcal{G}$ denote the collection of all undirected graphs, two of them being the same if they are isomorphic. A *graph invariant* is any function $f : \mathcal{G} \to \mathbb{C}$. We consider a special class of graph invariants, namely partition functions of spin models, defined as follows.

Let $n \in \mathbb{Z}_+$. Following de la Harpe and Jones [4], call any symmetric matrix $A \in \mathbb{C}^{n\times n}$ a *spin model* (over $\mathbb{C}$), with n *states*. The *partition function* of A is the function $p_A : \mathcal{G} \to \mathbb{C}$ defined for any graph $G = (V, E)$ by

(1) $$p_A(G) := \sum_{\kappa:V\to[n]} \prod_{uv\in E} A_{\kappa(u),\kappa(v)}.$$

Here and below, for $n \in \mathbb{Z}_+$,

(2) $$[n] := \{1, \ldots, n\}.$$

If G has k parallel vertices connecting u and v, the factor $A_{\phi(u),\phi(v)}$ occurs k times in (1).

The graph invariants p_A are motivated by parameters coming from mathematical physics and from graph theory. For instance, the Ising model corresponds to the matrix

(3) $$A = \begin{pmatrix} \exp(R/kT) & \exp(-R/kT) \\ \exp(-R/kT) & \exp(R/kT) \end{pmatrix},$$

where R is a positive constant, k is the Boltzmann constant, and T is the temperature. We refer to [1], [4], and [9] for motivation and more examples, and to [3], [5], [6], and [7] for related work and background.

In [7], partition functions of spin models were characterized in terms of certain Moebius transforms of graphs. In the present paper, we characterize these graph invariants in terms of the rank growth of associated 'connection matrices'. Rank growth of related connection matrices (but for 'k-labeled graphs') together with positive semidefiniteness was considered

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in Freedman, Lovász, and Schrijver [3] to characterize spin functions of real vertex models with weights on the states.

We describe the characterization. A *k-marked graph* is a pair (G, μ) of a graph $G = (V, E)$ and a function $\mu : [k] \to V$. We call $i \in [k]$ a *mark* of vertex $\mu(i)$. (We do not require that μ is injective, like for *k-labeled* graphs. So a vertex may have several marks.) Let $\mathcal{G}_k$ be the collection of k-marked graphs.

If (G, μ) and (H, ν) are k-marked graphs, then $(G, \mu)(H, \nu)$ is defined to be the graph obtained from the disjoint union of G and H by identifying equally marked vertices in G and H. (Another way of describing this is that we take the disjoint union of G and H, add edges connecting $\mu(i)$ and $\nu(i)$, for $i = 1, \ldots, k$, and finally contract each of these new edges.)

Let $f : \mathcal{G} \to \mathbb{C}$ and $k \in \mathbb{Z}_+$. The *k-th connection matrix* is the $\mathcal{G}_k \times \mathcal{G}_k$ matrix $C_{f,k}$ defined by

$$(4) \qquad (C_{f,k})_{(G,\mu),(H,\nu)} := f((G, \mu)(H, \nu))$$

for $(G, \mu), (H, \nu) \in \mathcal{G}_k$.

By $\emptyset$ we denote the graph with no vertices and edges. We can now formulate the characterization.

Theorem 1. *Let $f : \mathcal{G} \to \mathbb{C}$. Then $f = p_A$ for some symmetric $A \in \mathbb{C}^{n\times n}$ and some $n \in \mathbb{Z}_+$ if and only if $f(\emptyset) = 1$ and there is a c such that for each k:* $\text{rank}(C_{f,k}) \leq c^k$.

Our proof utilizes the characterization of partition functions of spin models given in [7], which uses the Nullstellensatz. One may alternatively apply the techniques described in Freedman, Lovász, and Schrijver [3]. With these techniques one may also extend Theorem 1 to more general structures like directed graphs and hypergraphs.

A related theorem can be proved for the vertex model, where the roles of vertices and edges are interchanged, using the characterization given in Draisma, Gijswijt, Lovász, Regts, and Schrijver [2] — see [8].

2. Partitions

As preliminary to the proof of Theorem 1, we give a (most probably folklore) proposition on partitions. A *partition* of a set X is an (unordered) collection of pairwise disjoint nonempty subsets of X with union X. The sets in P are called the *classes* of P. So $|P|$ is the number of classes of P.

Let Π_n denote the collection of partitions of $[n]$. We put $P \leq Q$ if P is a refinement of Q, that is, if each class of P is contained in some class of Q. Then $(\Pi_n, \leq)$ is a lattice; we denote the join by $\vee$.

Let Z be the 'zeta matrix', i.e., the $\Pi_n \times \Pi_n$ matrix with $Z_{P,Q} := 1$ if $P \leq Q$ and $Z_{P,Q} := 0$ otherwise. Let $M := Z^{-1}$ (the 'Moebius matrix').

For $n \in \mathbb{Z}_+$ and $x \in \mathbb{C}$, we define the $\Pi_n \times \Pi_n$ matrix $P_n(x)$ by

$$(5) \qquad (P_n(x))_{P,Q} := x^{|P\vee Q|}$$

for $P, Q \in \Pi_n$.

Proposition 1. *$P_n(x)$ is singular if and only if $x \in \{0, 1, \ldots, n-1\}$.*

Proof. Indeed, $MP_n(x)M^{\mathsf{T}}$ is a diagonal matrix, with

$$(MP_n(x)M^{\mathsf{T}})_{P,Q} = \delta_{P,Q} x(x-1)\cdots(x-|P|+1) \tag{6}$$

for $P, Q \in \Pi_n$. Here $\delta_{P,Q} = 1$ if $P = Q$ and $\delta_{P,Q} = 0$ otherwise. To prove (6), we can assume $x \in \mathbb{Z}_+$, as both sides are polynomials. For $\phi : [n] \to [x]$, let U_ϕ be the partition

$$U_\phi := \{\phi^{-1}(i) \mid i \in [x], \phi^{-1}(i) \neq \emptyset\}. \tag{7}$$

Then, where R and S range over Π_n:

$$\begin{aligned}(MP_n(x)M^{\mathsf{T}})_{P,Q} &= \sum_{R,S} M_{P,R} M_{Q,S} x^{|R\vee S|} = \sum_{R,S} M_{P,R} M_{Q,S} \sum_{\substack{\phi:[n]\to[x] \\ R\vee S \leq U_\phi}} 1 = \\ &\sum_{R,S} M_{P,R} M_{Q,S} \sum_{\substack{\phi:[n]\to[x] \\ R,S \leq U_\phi}} 1 = \sum_{\phi:[n]\to[x]} \Big(\sum_{R\leq U_\phi} M_{P,R}\Big)\Big(\sum_{S\leq U_\phi} M_{Q,S}\Big) = \\ &\sum_{\phi:[n]\to[x]} \delta_{P,U_\phi}\delta_{Q,U_\phi} = \delta_{P,Q} \sum_{\phi:[n]\to[x]} \delta_{P,U_\phi} = \delta_{P,Q} x(x-1)\cdots(x-|P|+1).\end{aligned} \tag{8}$$

∎

3. Proof of Theorem 1

Necessity is easy, and can be seen as follows. Let A be a symmetric $n \times n$ matrix, define $f := p_A$, and let $k \in \mathbb{Z}_+$. For any k-marked graph (G, μ) and any function $\lambda : [k] \to [n]$, define

$$B_{(G,\mu),\lambda} = \sum_{\substack{\kappa:V\to[n] \\ \kappa\circ\mu=\lambda}} \prod_{uv\in E} A_{\kappa(u),\kappa(v)}, \tag{9}$$

where $G = (V, E)$. This defines the $\mathcal{G}_k \times [n]^{[k]}$ matrix B, of rank at most n^k. Then $C_{f,k} = BB^{\mathsf{T}}$, so $C_{f,k}$ has rank at most n^k. This shows necessity.

We next show sufficiency. First observe that the conditions imply that

$$f(G \,\dot\cup\, H) = f(G)f(H) \tag{10}$$

for all $G, H \in \mathcal{G}$, where $G \,\dot\cup\, H$ denotes the disjoint union of G and H. This follows from the facts that the submatrix

$$\begin{pmatrix} f(\emptyset) & f(G) \\ f(H) & f(G \,\dot\cup\, H) \end{pmatrix} \tag{11}$$

of $C_{f,0}$ has rank at most 1 and that $f(\emptyset) = 1$.

By Theorem 1 in [7] it suffices to show that for any graph $G = (V, E)$ with $V = [k]$ and $k > f(K_1)$ one has

$$(12) \qquad \sum_{P \in \Pi_k} \mu_P f(G/P) = 0,$$

where $\mu_P := M_{T,P}$ (with M the Moebius matrix above), where T denotes the trivial partition of $[k]$ into singletons, and where G/P is the graph obtained from G by merging each class of P to one vertex (possibly creating several loops and multiple edges).

To prove (12), from here on we fix an integer $k > f(K_1)$. We can consider $\mathcal{G}_k$ as a commutative semigroup, by maintaining the marks in the product $(G, \mu)(H, \nu)$. The semigroup has a unity, namely the k-marked graph $\mathbf{1}_k$ with no edges and k distinct vertices marked $1, \ldots, k$.

Let $\mathbb{C}\mathcal{G}_k$ be the semigroup algebra of $\mathcal{G}_k$. We can extend f linearly to $\mathbb{C}\mathcal{G}_k$. Let $\mathcal{I}$ be the kernel of the matrix $C_{f,k}$, which can be considered as a subset of $\mathbb{C}\mathcal{G}_k$. Then $x \in \mathcal{I}$ if and only if $f(xy) = 0$ for each $y \in \mathbb{C}\mathcal{G}_k$. Hence $\mathcal{I}$ is an ideal in $\mathbb{C}\mathcal{G}_k$, and $\mathcal{A} := \mathbb{C}\mathcal{G}_k/\mathcal{I}$ is a finite-dimensional commutative unital algebra with $\dim(\mathcal{A}) = \operatorname{rank}(C_{f,k})$. Moreover, as f is 0 on $\mathcal{I}$, f has a (linear) quotient function $\hat{f}$ on $\mathcal{A}$. By definition of $\mathcal{I}$, for each nonzero $a \in \mathcal{A}$ there is a $b \in \mathcal{A}$ with $\hat{f}(ab) \neq 0$.

As $|\Pi_n|$ grows superexponentially in n, there exists an n such that $|\Pi_n| > c^{kn}$. Fix an (arbitrary) bijection $s : [k] \times [n] \to [kn]$. For each $P \in \Pi_n$ and $z \in \mathbb{C}\mathcal{G}_k$, let $\gamma_P(z)$ be the following element of $\mathbb{C}\mathcal{G}_{kn}$. For each $C \in P$, let z_C be a copy of z. For each $i \in [k]$ and $j \in [n]$ assign mark $s(i, j)$ to the vertex of z_C that was marked i in the original z, where C is the class of P containing j.

Using (10), it is direct to check that for any $P, Q \in \Pi_n$:

$$(13) \qquad f(\gamma_P(\mathbf{1}_k)\gamma_Q(z)) = \prod_{D \in P \vee Q} f(z^{\text{number of classes of } Q \text{ contained in } D}).$$

Proposition 2. *$\mathcal{A}$ is semisimple.*

Proof. As $\mathcal{A}$ is commutative and finite-dimensional, it suffices to show that any nilpotent element is zero. To this end, suppose $a \in \mathcal{A}$ is nilpotent, with $a \neq 0$. We can assume that $a^2 = 0$. Then there is an $x \in \mathbb{C}\mathcal{G}_k$ with $x \notin \mathcal{I}$ and $x^2 \in \mathcal{I}$. As $x \notin \mathcal{I}$, $f(xy) \neq 0$ for some $y \in \mathbb{C}\mathcal{G}_k$. Let $z := xy$. Then $f(z) \neq 0$ and $z^2 \in \mathcal{I}$. So $f(z^t) = 0$ for all $t \geq 2$. By scaling, we can assume that $f(z) = 1$.

Then for any $P, Q \in \Pi_n$ we have by (13)

$$(14) \qquad f(\gamma_P(\mathbf{1}_k)\gamma_Q(z)) = Z_{P,Q}.$$

As Z is nonsingular, this implies $\operatorname{rank}(C_{f,kn}) \geq |\Pi_n|$, contradicting the fact that $\operatorname{rank}(C_{f,kn}) \leq c^{kn} < |\Pi_n|$. ∎

Hence $\mathcal{A} \cong \mathbb{C}^t$, where $t = \dim(\mathcal{A})$.

Proposition 3. *If a is a nonzero idempotent in $\mathcal{A}$, then $\hat{f}(a)$ is a positive integer.*

Proof. Let $a = z + \mathcal{I}$ with $z \in \mathbb{C}\mathcal{G}_k$. So $f(z^t) = f(z)$ for all $t \geq 1$ (as $a^t = a$). Then for all $P, Q \in \Pi_n$ we have by (13)

$$f(\gamma_P(\mathbf{1}_k)\gamma_Q(z)) = (f(z))^{|P \vee Q|}. \tag{15}$$

As $|\Pi_n| > \operatorname{rank}(C_{f,kn})$, this implies that the matrix $P_n(f(z))$ is singular. So, by Proposition 1, $f(z) \in \mathbb{Z}_+$, and hence $\hat{f}(a) \in \mathbb{Z}_+$.

Suppose finally that a is a nonzero idempotent with $\hat{f}(a) = 0$. Then we can assume that a is a minimal nonzero idempotent. Hence ab is a scalar multiple of a for each b. So $\hat{f}(ab) = 0$ for each $b \in \mathcal{A}$, hence $a = 0$. ∎

For any partition P of $[k]$, let N_P be the k-marked graph with vertex set P, no edges, and where mark $i \in [k]$ is given to the element of P that contains i. Define the element b of $\mathbb{C}\mathcal{G}_k$ by

$$b := \sum_{P \in \Pi_k} \mu_P N_P, \tag{16}$$

where, as above,$\mu_P = M_{T,P}$ for all $P \in \Pi_k$ and T is the partition of $[k]$ consisting of singletons.

Proposition 4. *b is an idempotent in $\mathbb{C}\mathcal{G}_k$.*

Proof. First note that $N_P N_Q = N_{P \vee Q}$. Moreover, for each $R \in \Pi_k$:

$$\sum_{\substack{P,Q \in \Pi_k \\ P \vee Q = R}} \mu_P \mu_Q = \mu_R. \tag{17}$$

This follows from the uniqueness of μ, since for each $S \in \Pi_k$ we have, using $\mu_P = M_{T,P}$,

$$\sum_{R \leq S} \Big(\sum_{\substack{P,Q \in \Pi_k \\ P \vee Q = R}} \mu_P \mu_Q \Big) = \sum_{\substack{P,Q \in \Pi_k \\ P \vee Q \leq S}} \mu_P \mu_Q = \Big(\sum_{P \leq S} \mu_P \Big)^2 = (\delta_{T,S})^2 = \delta_{T,S}. \tag{18}$$

Since MZ is the identity matrix, (17) follows. Hence

$$b^2 = \sum_{P,Q \in \Pi_k} \mu_P \mu_Q N_{P \vee Q} = \sum_R \sum_{\substack{P,Q \in \Pi_k \\ P \vee Q = R}} \mu_P \mu_Q N_R = \sum_R \mu_R N_R = b. \tag{19}$$ ∎

Now, for any $x \in \mathbb{C}$,

$$(20) \qquad \sum_{P\in\Pi_k} \mu_P x^{|P|} = x(x-1)\cdots(x-k+1)$$

(cf. [7] — it also can be derived from (6) and (17)). Hence

$$(21) \qquad f(b) = \sum_{P\in\Pi_k} \mu_P f(N_P) = \sum_{P\in\Pi_k} \mu_P f(K_1)^{|P|} = f(K_1)(f(K_1)-1)\cdots(f(K_1)-k+1) = 0.$$

The last equality follows from the facts that $f(K_1)$ is a nonnegative integer and that $f(K_1) < k$. So $f(b) = 0$, and hence by Proposition 3, $b \in \mathcal{I}$.

Finally, to prove (12), consider any graph G with k vertices, say with vertex set $[k]$. Let vertex $i \in [k]$ be marked by i. Since $b \in \mathcal{I}$ we have $f(bG) = 0$. This is equivalent to (12), and finishes the proof of Theorem 1.

4. Final remark

The condition in the theorem says that $\log(\text{rank}(C_{f,k})) = O(k)$. The proof shows that it can be relaxed to $\log(\text{rank}(C_{f,k})) = o(k \log k)$, while keeping the conditions that $\text{rank}(C_{f,0}) = 1$ and $f(\emptyset) = 1$. This follows from the fact that if $\log(\text{rank}(C_{f,k})) = o(k \log k)$, then for each k there exists an n with $|\Pi_n| > \text{rank}(C_{f,kn})$. This is the property used in the proofs of Propositions 2 and 3.

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