ON THE WIDOM-ROWLINSON OCCUPANCY FRACTION IN REGULAR GRAPHS

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Abstract. We consider the Widom-Rowlinson model of two types of interacting particles on $d$-regular graphs. We prove a tight upper bound on the occupancy fraction: the expected fraction of vertices occupied by a particle under a random configuration from the model. The upper bound is achieved uniquely by unions of complete graphs on $d + 1$ vertices, $K_{d+1}$'s. As a corollary we find that $K_{d+1}$ also maximizes the normalized partition function of the Widom-Rowlinson model over the class of $d$-regular graphs. A special case of this shows that the normalized number of homomorphisms from any $d$-regular graph $G$ to the graph $H_{WR}$, a path on three vertices with a self-loop on each vertex, is maximized by $K_{d+1}$. This proves a conjecture of Galvin.

1. The Widom-Rowlinson Model

A Widom-Rowlinson assignment or configuration on a graph $G$ is a map $\chi : V(G) \to \{0, 1, 2\}$ so that 1 and 2 are not assigned to neighboring vertices, or in other words, a graph homomorphism from $G$ to the graph $H_{WR}$ consisting of a path on 3 vertices with a self-loop on each vertex (the middle vertex represents the label 0). Call the set of all such assignments $\Omega(G)$. The Widom-Rowlinson model on $G$ is a probability distribution over $\Omega(G)$ parameterized by $\lambda \in (0, \infty)$, given by:

$$\Pr[\chi] = \frac{\lambda^{X_1(\chi)+X_2(\chi)}}{P_G(\lambda)},$$

where $X_i(\chi)$ are the number of vertices colored $i$ under $\chi$, and

$$P_G(\lambda) = \sum_{\chi \in \Omega(G)} \lambda^{X_1(\chi)+X_2(\chi)}$$

is the partition function. Evaluating $P_G(\lambda)$ at $\lambda = 1$ counts the number of homomorphisms from $G$ to $H_{WR}$. We think of vertices assigned 1 and 2 as “colored” and those assigned 0 as “uncolored” (see Figure 1).

The Widom-Rowlinson model was introduced by Widom and Rowlinson in 1970 [13], as a model of two types of interacting particles with a hard-core exclusion between particles.

![Figure 1. A configuration for the Widom-Rowlinson model on a grid. Vertices mapping to 1 and 2 are shown as squares and diamonds, respectively (corresponding to Figure 2).](image-url)
of different types: color 1 and 2 represent particles of each type and color 0 represents an unoccupied site. The model has been studied both on lattices [9] and in the continuum [11, 2] and is known to exhibit a phase transition in both cases.

The Widom-Rowlinson model is one case of a general random model: that of choosing a random homomorphism from a large graph $G$ to a fixed graph $H$. In the Widom-Rowlinson case, we take $H = H_{\text{WR}}$. Another notable case is $H_{\text{ind}}$, an edge between two vertices, one of which has a self loop (see Figure 2). Homomorphisms from $G$ to $H_{\text{ind}}$ are exactly the independent sets of $G$, and the partition function of the hard-core model is the sum of $\lambda^{|I|}$ over all independent sets $I$. An overview of the connections between statistical physics models with hard constraints, graph homomorphisms, and combinatorics can be found in [1].

For every such model, there is an associated extremal problem. Denote by $\text{hom}(G, H)$ the number of homomorphisms from $G$ to $H$. Then we can ask which graph $G$ from a class of graphs $\mathcal{G}$ maximizes $\text{hom}(G, H)$, or if we wish to compare graphs on different numbers of vertices, ask which graph maximizes the scaled quantity $\text{hom}(G, H)|V(G)|/|\lambda|$. Kahn [8] proved that for any $d$-regular, bipartite graph $G$,

$$\text{hom}(G, H_{\text{ind}}) \leq \text{hom}(K_{d,d}, H_{\text{ind}})|V(G)|/2d,$$

where $K_{d,d}$ is the complete $d$-regular bipartite graph. Equality holds in (1) if $G$ is $K_{d,d}$ or a union of $K_{d,d}$'s. In other words, unions of $K_{d,d}$'s maximize the total number of independent sets over all $d$-regular, bipartite graphs on a fixed number of vertices.

In a broad generalization of Kahn’s result, Galvin and Tetali [7] showed that in fact, (1) holds for all $d$-regular, bipartite $G$ and all target graphs $H$ (including, for example, $H_{\text{WR}}$). And using a cloning construction and a limiting argument, they showed that in fact the partition function of such models (a weighted count of homomorphisms) is maximized by $K_{d,d}$; for example, for a $d$-regular, bipartite $G$,

$$P_G(\lambda) \leq P_{K_{d,d}}(\lambda)|V(G)|/2d,$$

where $P_G(\lambda)$ is the Widom-Rowlinson partition function defined above or the independence polynomial of a graph. Note that the case $\lambda = 1$ is the counting result.

There is no such sweeping statement for the class of all $d$-regular graphs with the bipartiteness restriction removed. In [14] and [15], Zhao showed that the bipartiteness restriction on $G$ in (1) and (2) can be removed for some class of graphs $H$, including $H_{\text{ind}}$. But such an extension is not possible for all graphs $H$; for example, $K_{d+1}$ has more homomorphisms to $H_{\text{WR}}$ than does $K_{d,d}$ (after normalizing for the different numbers of vertices). In fact Galvin conjectured the following:

**Conjecture 1** (Galvin [5, 6]). Let $G$ be a any $d$-regular graph. Then

$$\text{hom}(G, H_{\text{WR}}) \leq \text{hom}(K_{d+1}, H_{\text{WR}})|V(G)|/(d+1).$$
The more general Conjecture 1.1 of [5] that the maximizing $G$ for any $H$ is either $K_{d,d}$ or $K_{d+1}$ has been disproved by Sernau [12].

The above theorems of Kahn and Galvin and Tetali are based on the entropy method (see [10] and [6] for a survey), but in this context bipartiteness seems essential for the effectiveness of the method. We will approach the problem differently, using the occupancy method of [3].

We first define the occupancy fraction $\alpha_G(\lambda)$ to be the expected fraction of vertices which receive a (nonzero) color in the Widom-Rowlinson model:

$$\alpha_G(\lambda) = \frac{E[X_1 + X_2]}{|V(G)|},$$

where $X_i$ is the number of vertices colored $i$ by the random assignment $\chi$. A calculation shows that $\alpha_G(\lambda)$ is in fact the scaled logarithmic derivative of the partition function:

$$\alpha_G(\lambda) = \frac{\lambda |V(G)| \cdot \frac{P_G'(\lambda)}{P_G(\lambda)} = \frac{\lambda \cdot (\log P_G(\lambda))'}{|V(G)|}}.$$

Our main result is that for any $\lambda$, $\alpha_G(\lambda)$ is maximized over all $d$-regular graphs $G$ by $K_{d+1}$.

**Theorem 1.** Let $G$ be any $d$-regular graph and $\lambda > 0$. Then

$$\alpha_G(\lambda) \leq \alpha_{K_{d+1}}(\lambda)$$

with equality if and only if $G$ is a union of $K_{d+1}$’s.

We will prove this by introducing local constraints on random configurations induced by the Widom-Rowlinson model on a $d$-regular graph $G$, then solving a linear programming relaxation of the optimization problem over all $d$-regular graphs.

Theorem 1 implies maximality of the normalized partition function:

**Corollary 1.** Let $G$ be a $d$-regular graph and $\lambda > 0$. Then

$$\frac{1}{|V(G)|} \log P_G(\lambda) \leq \frac{1}{d+1} \log P_{K_{d+1}}(\lambda),$$

or equivalently,

$$P_G(\lambda) \leq P_{K_{d+1}}(\lambda)^{|V(G)|/(d+1)},$$

with equality if and only if $G$ is a union of $K_{d+1}$’s.

The quantity $\frac{1}{|V(G)|} \log P_G(\lambda)$ is known in statistical physics as the free energy per unit volume. Corollary 1 follows from Theorem 1 as follows: $\frac{1}{|V(G)|} \log P_G(0) = 0$ for any $G$, and so

$$\frac{1}{|V(G)|} \log P_G(\lambda) = \frac{1}{|V(G)|} \int_0^\lambda (\log P_G(t))' \, dt \leq \frac{1}{d+1} \int_0^\lambda (\log P_{K_{d+1}}(t))' \, dt = \frac{1}{d+1} \log P_{K_{d+1}}(\lambda)$$

where the inequality follows from Theorem 1 and (3). Exponentiating both sides gives Corollary 1.

By taking $\lambda = 1$ in Corollary 1, we get the counting result:
Corollary 2. For all $d$-regular $G$,

$$\text{hom}(G, H_{\text{WR}}) \leq \text{hom}(K_{d+1}, H_{\text{WR}})^{|V(G)|/(d+1)}$$

with equality if and only if $G$ is a union of $K_{d+1}$'s.

This proves Conjecture 1.

Discussion and related work. The method we use is more probabilistic than the entropy method in the sense that Theorem 1 gives information about an observable of the model; in some statistical physics models, the analogue of $\alpha_G(\lambda)$ would be called the mean magnetization. We also work directly in the statistical physics model, instead of counting homomorphisms.

Davies, Jenssen, Perkins, and Roberts [3] applied the occupancy method to two central models in statistical physics: the hard-core model of a random independent set described above, and the monomer-dimer model of a randomly chosen matching from a graph $G$. In both cases they showed that $K_{d,d}$ maximizes the occupancy fraction over all $d$-regular graphs. In the case of independent sets this gives a strengthening of the results of Kahn, Galvin and Tetali, and Zhao, while for matchings, it was not known previously that unions of $K_{d,d}$ maximizes the partition function or the total number of matchings.

The idea of calculating the log partition function by integrating a partial derivative is not new of course; see for example, the interpolation scheme of Dembo, Montanari, and Sun [4] in the context of Gibbs distributions on locally tree-like graphs. The method is powerful because it reduces the computation of a very global quantity, $P_G(\lambda)$, to that of a locally estimable quantity, $\alpha_G(\lambda)$.

Some partial results towards the Widom-Rowlinson counting problem were obtained by Galvin [5], who showed that a graph with more homomorphisms than a union of $K_{d+1}$'s must be close in a specific sense to a union of $K_{d+1}$'s.

2. Proof of Theorem 1

2.1. Preliminaries. To prove Theorem 1, we will use the following experiment: for a $d$-regular graph $G$, we first draw a random $\chi$ from the Widom-Rowlinson model, then select a vertex $v$ uniformly at random from $V(G)$. We then write our objective function, the occupancy fraction, in terms of local probabilities with respect to this experiment, and add constraints on the local probabilities that must hold for all $G$. We then relax the optimization problem to all distributions satisfying the local constraints, and optimize using linear programming.

Fix $d$ and $\lambda$. Define a configuration with boundary conditions $C = (H, \mathcal{L})$ to be a graph $H$ on $d$ vertices with family of lists $\mathcal{L} = \{L_u\}_{u \in H}$, where each $L_u \subseteq \{1, 2\}$ is a set of allowed colors for the vertex $u$. Here $H$ represents the neighborhood structure of a vertex $v \in V(G)$ and the color lists $L_u$ represent the colors permitted to neighbors of $v$, given an assignment $\chi$ on the vertices outside of $N(v) \cup \{v\}$. (See Figure 3.) Denote by $\mathcal{C}$ the set of all possible configurations with boundary conditions in any $d$-regular graph.

We now pick the assignment $\chi$ at random from the Widom-Rowlinson model on a fixed $d$-regular graph $G$, pick a vertex $v$ uniformly at random from $V(G)$, and consider the probability distribution induced on $\mathcal{C}$. 
Figure 3. An example configuration with boundary conditions based on a coloring $\chi$. The graph $H$ consists of the four neighbors of $v$ along with the black edges, and the list $L_u$ is shown above each vertex $u$ of $H$. The colors assigned by $\chi$ to $v$ and its neighbors are immaterial and so are not shown.

For example, if $G = K_{d+1}$ then with probability 1 the random configuration $C$ is $H = K_d$ with $L_u = \{1, 2\}$ for all $u \in V(H)$. If $G = K_{d,d}$ then $H$ is always $d$ isolated vertices and the color lists can be any (possibly empty) subset of $\{1, 2\}$, but the lists must be the same for all $u \in V(H)$.

For a configuration $C = (H, L)$, define

$$\alpha^v_i(C) = \Pr[\chi(v) = i | C]$$
$$\alpha^u_i(C) = \frac{1}{d} \sum_{u \in V(H)} \Pr[\chi(u) = i | C],$$

where the probability is over the Widom-Rowlinson model on $G$ given the boundary conditions $L$. Note that the spatial Markov property of the model means that these probabilities are “local” in the sense that they can be computed knowing only $C$. Let $\alpha^v(C) = \alpha^v_1(C) + \alpha^v_2(C)$ and $\alpha^u(C) = \alpha^u_1(C) + \alpha^u_2(C)$. Then we have

$$\alpha_G(\lambda) = \frac{1}{|V(G)|} \sum_{v \in V(G)} \Pr[\chi(v) \in \{1, 2\}] = \mathbb{E}_C[\alpha^v(C)]$$
$$= \frac{1}{d |V(G)|} \sum_{v \in V(G)} \sum_{u \sim v} \Pr[\chi(u) \in \{1, 2\}] = \mathbb{E}_C[\alpha^u(C)],$$

where the expectations are over the probability distribution induced on $C$ by our experiment of drawing $\chi$ from the model and $v$ uniformly at random from $V(G)$, and the last sum is over all neighbors of $v$ in $G$. Equality of the two expressions for $\alpha$ follows since sampling a uniform neighbor or a uniform vertex in a regular graph is equivalent to sampling a uniform vertex. We will show that this expectation is maximized when the graph $G$ is $K_{d+1}$.

We can in fact write explicit formulae for $\alpha^v(C)$ and $\alpha^u(C)$. For a configuration $C = (H, L)$, let $P_C^{(0)}(\lambda)$ be the total weight of colorings of $H$ satisfying the boundary conditions given by the lists $L$ (corresponding to the partition function for the neighborhood of $v$ conditioned on $\chi(v) = 0$). Also, write $P_C^{(i)}(\lambda)$ for the total weight of colorings of $H$ satisfying the boundary conditions and using only color $i$ and 0 (corresponding to the partition functions for the neighborhood of $v$ conditioned on $\chi(v) = i$). Finally, let $P_C^{(12)}(\lambda) = P_C^{(1)}(\lambda) + P_C^{(2)}(\lambda)$ and let

$$P_C(\lambda) = P_C^{(0)}(\lambda) + \lambda P_C^{(12)}(\lambda)$$
be the partition function of \( N(v) \cup \{v\} \) conditioned on the boundary conditions given by \( \mathcal{C} \).

Note that if \( \mathcal{L} \) has \( a_1 \) lists containing 1 and \( a_2 \) lists containing 2, then \( P_C^{(i)}(\lambda) = (1 + \lambda)^{a_i} \).

Now we can write
\[
\alpha^v(C) = \frac{\lambda P_C^{(12)}}{P_C} \quad \text{and} \quad \alpha^u(C) = \frac{\lambda \left( P_C^{(0)'} + \lambda (P_C^{(12)})' \right)}{d P_C},
\]

where \( P' \) is the derivative of \( P \) in \( \lambda \). We will suppress the dependence of the partition functions on \( \lambda \) from now on.

For \( G = K_{d+1} \), we have
\[
P_{K_{d+1}} = 2(1 + \lambda)^{d+1} - 1 \quad \text{and} \quad \alpha_{K_{d+1}}(\lambda) = \frac{2\lambda(1 + \lambda)^d}{2(1 + \lambda)^{d+1} - 1}.
\]

If \( G = K_{d+1} \) then the only possible configuration is \( C_{K_{d+1}} \), the complete neighborhood \( K_d \) with full boundary lists, so we also have \( \alpha^v(K_d) = \alpha^u(K_d) = \alpha_{K_{d+1}}(\lambda) \) (we can also compute these directly). Since this quantity will arise frequently, we will use the notation \( \alpha_K = \alpha_{K_{d+1}}(\lambda) \).

### 2.2. A linear programming relaxation.

Now let \( q : \mathcal{C} \rightarrow [0,1] \) denote a probability distribution over the set of all possible configurations. Then we set up the following optimization problem over the variables \( q(C), \ C \in \mathcal{C} \).

\[
\alpha^* = \max \sum_{C \in \mathcal{C}} q(C) \alpha^v(C) \quad \text{s.t.}
\]
\[
\sum_{C \in \mathcal{C}} q(C) = 1 \quad \sum_{C \in \mathcal{C}} q(C)[\alpha^v(C) - \alpha^u(C)] = 0 \quad q(C) \geq 0 \quad \forall C \in \mathcal{C}.
\]

Note that this linear program is indeed a relaxation of our optimization problem of maximizing \( \alpha_G(\lambda) \) over all \( d \)-regular graphs: any such graph induces a probability distribution on \( \mathcal{C} \), and as we have seen above in (4), the constraint asserting the equality \( \mathbb{E} \alpha^v(C) = \mathbb{E} \alpha^u(C) \) must hold in all \( d \)-regular graphs.

We will show that for any \( \lambda > 0 \) the unique optimal solution of this linear program is \( \alpha(C_{K_{d+1}}) = 1 \), where \( C_{K_{d+1}} \) is the configuration induced by \( K_{d+1} : H = K_d \) and \( L_u = \{1, 2\} \) for all \( u \in H \).

The dual of the above linear program is
\[
\alpha^* = \min \Lambda_p \quad \text{s.t.}
\]
\[
\Lambda_p + \Lambda_c(\alpha^v(C) - \alpha^u(C)) \geq \alpha^v(C) \quad \forall C \in \mathcal{C},
\]

with decision variables \( \Lambda_p \) and \( \Lambda_c \).

To show that the optimum is attained by \( C_{K_{d+1}} \), we must find a feasible solution to the dual program with \( \Lambda_p = \alpha_K = \frac{2\lambda(1 + \lambda)^d}{2(1 + \lambda)^{d+1} - 1} \). Note that with \( \Lambda_p = \alpha_K \) the constraint for \( C_{K_{d+1}} \) holds with equality for any choice of \( \Lambda_c \). In other words, it suffices to find some convex
combination of the two local estimates $\alpha^u$ and $\alpha^v$ which is maximized by $C_{K_{d+1}}$ over all $C \in \mathcal{C}$.

Let $C_0$ be a configuration with $L_u = \emptyset$ for all $u \in H$ (in which case the edges of $H$ are immaterial, and so abusing notation we will refer to any one of these configurations as $C_0$). We find a candidate $\Lambda_c$ by solving the constraint corresponding to $C_0$ with equality:

$$\alpha_K = \Lambda_c(\alpha^u(C_0) - \alpha^v(C_0)) + \alpha^v(C_0)$$

$$= (1 - \Lambda_c)\frac{2\lambda}{1 + 2\lambda}.$$

This gives

$$\Lambda_c = 1 - \frac{\alpha_K}{2\lambda}(1 + 2\lambda) = \frac{\alpha_K}{2\lambda} \frac{(1 + \lambda)^d - 1}{(1 + \lambda)^d}.$$

With this choice of $\Lambda_c$, the general dual constraint is

$$\alpha_K \geq \frac{\alpha_K}{2\lambda} \frac{(1 + \lambda)^d - 1}{(1 + \lambda)^d} \alpha^u(C) + \frac{\alpha_K}{2\lambda} (1 + 2\lambda) \alpha^v(C).$$

Using (5), this becomes

$$(7) \quad \frac{(P_C^{(0)})' + \lambda(P_C^{(12)})'}{2P_C^{(0)} - P_C^{(12)}} \leq \frac{d(1 + \lambda)^d}{(1 + \lambda)^d - 1}.$$

From this point on we may assume that $C$ has some non-empty color list, since otherwise the configuration is equivalent to $C_0$ and the constraint holds with equality by our choice of $\Lambda_c$. This assumption tells us, among other things, that $(P_C^{(0)})' > 0$ and $2P_C^{(0)} - P_C^{(12)} > 0$.

Our goal is now to show that (7) holds for all $C$. We consider the two terms separately.

**Claim 1.** For any $C \neq C_0$,

$$\frac{\lambda(P_C^{(12)})'}{2P_C^{(0)} - P_C^{(12)}} \leq \frac{d\lambda(1 + \lambda)^{d-1}}{(1 + \lambda)^d - 1},$$

with equality if and only if the lists $L_u$ are all equal and $C$ has no dichromatic colorings.

**Proof.** Since the partition function $P_C^{(0)}$ is at least the total weight $P_C^{(1)} + P_C^{(12)} - 1$ of monochromatic colorings (with equality when $C$ has no dichromatic colorings), we have

$$(8) \quad \frac{(P_C^{(12)})'}{2P_C^{(0)} - P_C^{(12)}} \leq \frac{(P_C^{(12)})'}{P_C^{(12)} - 2} = \frac{a_1(1 + \lambda)^{a_1-1} + a_2(1 + \lambda)^{a_2-1}}{(1 + \lambda)^{a_1} + (1 + \lambda)^{a_2} - 2}$$

(where, as above, $a_i$ is the number of vertices in $H$ allowed color $i$ under the given boundary conditions), and so we need to show that

$$\frac{a_1(1 + \lambda)^{a_1-1} + a_2(1 + \lambda)^{a_2-1}}{(1 + \lambda)^{a_1} + (1 + \lambda)^{a_2} - 2} \leq \frac{d(1 + \lambda)^{d-1}}{(1 + \lambda)^d - 1}.$$

In general, to show that $(a+b)/(c+d) \leq t$ it suffices to show that $a/c \leq t$ and $b/d \leq t$. Thus it is enough to show that

$$(9) \quad \frac{a(1 + \lambda)^{a-1}}{(1 + \lambda)^a - 1} \leq \frac{d(1 + \lambda)^{d-1}}{(1 + \lambda)^d - 1}.$$
whenver $1 \leq a \leq d$. (Note that if either $a_1 = 0$ or $a_2 = 0$ then (8) reduces to (9), and if both $a_1, a_2 = 0$ then the configuration is $C_0$). Indeed, it is not hard to check via calculus that the left hand side of (9) is increasing with $a$. This completes the proof of the inequality in Claim 1.

We have equality in this final step when $a_1 = a_2 = d$ or when one is 0 and the other is $d$. So we have equality overall whenever the lists are all equal and there are no dichromatic colorings (recall that we are assuming $C$ has some non-empty coloring list). □

**Claim 2.** For any $C \neq C_0$,

$$\frac{(P_C^{(0)})'}{2P_C^{(0)} - P_C^{(12)}} \leq \frac{d(1 + \lambda)^{d-1}}{(1 + \lambda)^d - 1},$$

with equality if and only if the lists $L_u$ are all equal and $C$ has no dichromatic colorings.

**Proof.** We can write

$$\frac{\lambda(P_C^{(0)})'}{2P_C^{(0)} - P_C^{(12)}} = \frac{\lambda(P_C^{(0)})'}{P_C^{(0)} - (P_C^{(0)} - P_C^{(1))}) + (P_C^{(0)} - P_C^{(2))})} = \frac{E_C[X_1] + E_C[X_2]}{Pr_C[X_1 > 0] + Pr_C[X_2 > 0]},$$

where now $X_i$ is the number of vertices colored $i$ in a random coloring chosen from the Widom-Rowlinson model on $C$. Noting that $E_C[X_1] = 0$ whenever $Pr_C[X_1 > 0] = 0$, it suffices as above to show that whenever color 1 is permitted anywhere in $C$,

$$(10) \quad \frac{E_C[X_1]}{Pr_C[X_1 > 0]} = E_C[X_1 | X_1 > 0] \leq \frac{\lambda d(1 + \lambda)^{d-1}}{(1 + \lambda)^d - 1} = E_K[d | X_1 > 0],$$

and similarly for $X_2$, but this will follow by symmetry.

We can decompose the expectation as

$$E_C[X_1 | X_1 > 0] = \sum_{S \subseteq V(H)} Pr_C[X^{-1}(2) = S | X_1 > 0] \cdot E_C[X_1 | X_1 > 0 \land \chi^{-1}(2) = S].$$

The partition function restricted to colorings satisfying $X_1 > 0$ and $\chi^{-1}(2) = S$ is just $P_S(\lambda) = \lambda^{|S|}((1 + \lambda)^{a_S} - 1)$, where $a_S$ is the number of vertices in $H \setminus S$ which are allowed color 1 and are not adjacent to any vertex of $S$. The conditional expectation is then

$$E_C[X_1 | X_1 > 0 \land \chi^{-1}(2) = S] = \frac{a_S \lambda(1 + \lambda)^{a_S-1}}{(1 + \lambda)^{a_S} - 1} \leq \frac{d\lambda(1 + \lambda)^{d-1}}{(1 + \lambda)^d - 1},$$

with equality precisely when $S$ is empty and 1 is available for every vertex. That is,

$$E_C[X_1 | X_1 > 0] \leq \sum_{S \subseteq V(H)} Pr_C[X^{-1}(2) = S | X_1 > 0] \cdot \frac{d\lambda(1 + \lambda)^{d-1}}{(1 + \lambda)^d - 1} = \frac{\lambda d(1 + \lambda)^{d-1}}{(1 + \lambda)^d - 1},$$

as desired. We have equality in (10) when $Pr_C[a_S = d | X_1 > 0] = 1$, which holds for the configurations where 1 is available to every vertex but which have no dichromatic colorings. That is, for equality to hold in the claim $C$ must have no dichromatic colorings, and any color which is available to some vertex $u$ must be available to every vertex (so the lists must be identical). □
Adding the inequalities in Claims 2 and 1 shows that (7) holds for all $C$, proving optimality of $K_{d+1}$.

2.3. Uniqueness.

**Lemma 1.** The distribution induced by $K_{d+1}$ is the unique optimum of the LP relaxation (6).

**Proof.** Complementary slackness for our dual solution says that any optimal primal solution is supported only on configurations $C$ with identical boundary lists and no dichromatic colorings. These fall into three categories:

**Case 0:** $L_u = \emptyset$ for all $u$. In this case the edges of $H$ are immaterial, as none of $H$ can be colored. This is the configuration $C_0$ above.

**Case 1:** $L_u = \{i\}$ for all $u$ (for $i = 1$ or 2). The edges of $H$ are again immaterial, as every coloring of $H$ with only color $i$ is allowed. Call this configuration $C_1$.

**Case 2:** $L_u = \{1, 2\}$ for all $u$. In this case the prohibition on dichromatic colorings requires that $C = C_{K_{d+1}}$.

We can calculate $\alpha^v(C)$ and $\alpha^u(C)$ for each case. For Case 0 we have

$$\alpha^v(C_0) = \frac{2\lambda}{1 + 2\lambda} \quad \text{and} \quad \alpha^u(C_0) = 0.$$ 

For Case 1 we have

$$\alpha^v(C_1) = \frac{\lambda + \lambda(1 + \lambda)^d}{\lambda + (1 + \lambda)^{d+1}} \quad \text{and} \quad \alpha^u(C_1) = \frac{\lambda(1 + \lambda)^d}{\lambda + (1 + \lambda)^{d+1}}.$$ 

And of course, for Case 2 we have

$$\alpha^v(K_d) = \alpha^u(K_d) = \alpha_K.$$ 

In both Case 0 and Case 1 we have $\alpha^u < \alpha^v$, so the only convex combination $q$ of the three cases giving $\sum C q(C) \alpha^u(C) = \sum C q(C) \alpha^v(C)$ (as is required for feasibility) is the one which puts all of the weight on $C_{K_{d+1}}$. □

3. DISTINCT ACTIVITIES

It is also natural to consider a weighted version of the Widom-Rowlinson model with distinct activities $\lambda_1, \lambda_2$ for the two colors, so that the configuration $\chi$ is chosen with probability proportional to $\lambda_1^{X_1} \lambda_2^{X_2}$, and where the partition function $P_G(\lambda_1, \lambda_2)$ is again the normalizing factor. We can ask which graphs maximize $P(\lambda_1, \lambda_2)^{1/|V(G)|}$. We conjecture

**Conjecture 2.** For any $\lambda_1, \lambda_2 > 0$, the weighted occupancy fraction

$$\sigma_G(\lambda_1, \lambda_2) = \frac{\lambda_2 \alpha_1^G(\lambda_1, \lambda_2) + \lambda_1 \alpha_2^G(\lambda_1, \lambda_2)}{\lambda_1 + \lambda_2}$$

is maximized over all $d$-regular graphs by $K_{d+1}$.

In fact, Conjecture 2 implies the following conjecture on the maximality of the partition function:

**Conjecture 3.** For any $\lambda_1, \lambda_2 > 0$, and any $d$-regular graph $G$,

$$P_G(\lambda_1, \lambda_2) \leq P_{K_{d+1}}(\lambda_1, \lambda_2)^{|V(G)|/(d+1)}.$$
To see this, assume $\lambda_1 \geq \lambda_2$, and let $F_G(x) = \frac{1}{n} \log P_G(\lambda_1 - \lambda_2 + x, x)$. We have

$$
\frac{1}{n} \log P_G(\lambda_1, \lambda_2) = F_G(\lambda_2) = F_G(0) + \int_0^{\lambda_2} \frac{dF_G}{dx}(x) \, dx
$$

$F_G(0) = \frac{1}{n} \log P_G(\lambda_1 - \lambda_2, 0) = \log(1 + \lambda_1 - \lambda_2)$ for all graphs $G$, and so if we can show that for all $0 \leq x \leq \lambda_2$, $\frac{dF_G}{dx}(x)$ is maximized when $G = K_{d+1}$, then we obtain (the log of) inequality (11). We compute:

$$
\frac{dF_G}{dx}(x) = \frac{1}{n} \frac{d}{dx} P_G(\lambda_1 - \lambda_2 + x, x) = \frac{1}{n} \sum_x \frac{x X_1 + (\lambda_1 - \lambda_2 + x) X_2 (\lambda_1 - \lambda_2 + x) X_1 \cdot X_2}{P_G(\lambda_1 - \lambda_2 + x, x)}
$$

$$
= \frac{1}{x(\lambda_1 - \lambda_2 + x)} \left[ x\alpha_G(1)(\lambda_1 - \lambda_2 + x, x) + (\lambda_1 - \lambda_2 + x)\alpha_G(2)(\lambda_1 - \lambda_2 + x, x) \right]
$$

Conjecture 2 implies that this is maximized by $K_{d+1}$.

References


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