Counting without sampling. New algorithms for enumeration problems using statistical physics

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Abstract

We propose a new type of approximate counting algorithms for the problems of enumerating the number of independent sets and proper colorings in low degree graphs with large girth. Our algorithms are not based on a commonly used Markov chain technique, but rather are inspired by recent developments in statistical physics in connection with correlation decay properties of Gibbs measures and its implications to uniqueness of Gibbs measures on infinite trees, reconstruction problems and local weak convergence methods. On a negative side, our algorithms provide ϵ-approximations only to the logarithms of the size of a feasible set (also known as free energy in statistical physics). But on the positive side, unlike Markov chain based algorithms, our approach provides deterministic as opposed to probabilistic guarantee on approximations. Moreover, for some regular graphs we obtain explicit values for the counting problem. For example, we show that every 4-regular n-node graph with large girth has asymptotically $(1.494\ldots)^n$ independent sets, and in every r-regular graph with n nodes and large girth the number of $q \geq r+1$-proper colorings is asymptotically $(q(1-\frac{1}{q})^{\frac{r}{2}})^n$, for large n. In statistical physics terminology, we compute explicitly the partition function (free energy) in these cases. We extend our results to random regular graphs graphs also. The explicit results obtained in this paper would be hard to derive via Markov chain sampling technique.

1 Introduction

Counting is a natural counterpart to a combinatorial optimization problem. The most widely studied such problems involve counting the number of solutions to a bin packing problem [JS97], counting the number of independent sets (also known as hard-core model in statistical physics) [LV97],[DGJ04], matchings [JS97], proper colorings in graphs (Potts model) [DGJ04], [DFHV04], volume of a convex body [DaRK91],[KLS97], [LV03], permanent of a matrix [Val79],[JS89], [JSV04], [JS97], [BSVV] etc. Solving counting problems exactly seems intractable as Valiant [Val79] introduced $\#P$ complexity class which includes most of the interesting counting problems, and thus research efforts focused on approximation algorithms. Here the most powerful method comes from the theory of rapidly mixing Markov chains. The typical setup involves relating counting problem to a sampling problem via certain telescoping trick (see for example identity (2.1) below) and then computing some marginal probabilities using sampling technique. The main technical challenge is establishing that the underlying Markov chain mixes in polynomial time (rapid mixing) and this has been established for many very interesting counting problems including Jerrum and Sinclair's [JS89], and Jerrum, Sinclair and Vigoda's [JSV04] proof of rapid mixing of a Markov chain related to permanents, and Dyer, Frieze and Kannan [DaRK91] proof of rapid mixing of a Markov chain related to computing the volume of a convex body. Subsequent improvements in running time for computing volumes have been established in Kannan, Lovasz and Simonovits [KLS97] and Lovasz and Vempala [LV03]. Somewhat closer to the topic of this paper, Luby and Vigoda [LV97] showed that a Markov chain related to counting independent sets is rapidly mixing, when the underlying graph has degree at most 4.

A natural extension of the counting problem involves computing a partition function. Partition function is a fundamental object in statistical physics arising in connection with Gibbs distribution. Thus the connection between the counting problem and statistical physics is well known. There are many results in statistical physics literature on computing partition functions in various statistical physics models, but unfortunately, most of these results are not rigorous and involve what is known as replica-symmetry and replica symmetry breaking cavity method also known as replica symmetry breaking Ansatz [MPV87]. The process of rigorization of these spectacular but unproven results by physicists was undertaken relatively recently in mathematics. In particular Talgrand [Tal03] proved the validity of the Parisi formula for the partition function limit of a Sherrington-Kirpatrick's model. Also Talagrand [Tal01] proved the existence of the partition func-

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tion limit of a random K-SAT problem in an appropriately defined high temperature regime. However, the process of building a full mathematical picture of the cavity and replica-symmetry methods is still largely under way.

In this paper we propose new approach for solving the problems of counting the number of independent sets and proper colorings in some graphs. Our primary setting is low degree graphs with locally tree-like structure (large girth). In particular we propose a polynomial time algorithm for computing approximately the logarithm of the number of independent sets in graphs with maximum degree ≤ 4 and large girth (appropriately defined). Similarly, for every q we propose an algorithm for computing approximately the logarithm of the number of proper q-colorings of any graph with maximum degree $\leq q-1$ and large girth.

On a negative side our algorithms is only an approximation on the log scale: for every constant ϵ we compute ϵ-approximation of the log-partition function (also called free energy in statistical physics). Also our computation time, while polynomial in the size of the graph, is not polynomial in ϵ. Thus our algorithm is PAS (Polynomial Time Approximation Scheme) as opposed to FPRAS (Fully Polynomial Time Randomized Approximation Scheme) as is typical for Markov chains method. But there are two crucial advantages to our method. First, our algorithms are deterministic and thus the sampling error is removed. Second, in special cases involving regular graphs we obtain the values of the partition function *explicitly.* For example we show that in every 4-regular graph with n nodes and large girth, the number of independent sets is asymptotically $(1.494\ldots)^n$ *irrespectively of the graph!* The class of regular graphs with large girth is very rich and the fact that the number of independent sets is the same in all of them is an interesting by-product of our analysis. The value $1.494\ldots$ is a numeric approximation of a solution to a certain fixed-point equation. We obtain similar limiting numeric values for the case of r-regular graphs when $r = 2, 3, 4, 5$. For the problem of counting the number of proper colorings, we show that for every constant $q \geq r+1$, the number of q colorings in every r-regular graphs with large girth is asymptotically $(q(1-\frac{1}{q})^{\frac{r}{2}})^n$, when n is large. We note, that our results allow both q and r to be small. All of the known results for counting which are based on Markov chain method require q/r to be at least a large positive constant [DFHV04].

As a corollary of our main results, we compute the expected value of the free energy with respect to independent sets (hard-core) in random r-regular graphs when $r = 2, 3, 4, 5$ and, in particular, show that the limit of the expected free energy exists. Even establishing the existence of such limits is a highly non-trivial problem.

The main technical approach underlying our results is the progress in understanding properties of Gibbs distributions on regular infinite trees for independent sets, coloring, Ising and some other related models in the context of *correlation decay* and the connection of thereof to the uniqueness of Gibbs measure. We use this stream of work to propose a different method for computing marginal probability featuring in cavity equation (2.1) below. In one of the earliest results in this area, Kelly [Kel85] established the following phase transition property for independent set on infinite r-regular trees: the probability that a root of the tree belongs to an independent set selected according to the Gibbs measure is asymptotically independent from the finite depth boundary of a tree, provided that inverse temperature λ is sufficiently small. The "counting" case $\lambda = 1$ satisfies this condition for $r \leq 5$ but breaks down for larger r. A recent extension of this result to general Galton-Watson type random trees and Erdos-Renyie type random graphs was done by Bandyopadhyay [Ban]. Similar uniqueness property is also known for Ising model [Geo88] and recently was established for coloring in the case of $q \geq r+1$ colors by Jonasson [Jon02], closing an open problem posed earlier by Brightwell and Winkler [BW02]. The correlation decay property (long-range independence) featured lately very prominently in a variety of contexts including Aldous' proof of the ζ_2-limit forthe random assignment problem [Ald01], bivariate uniqueness and endogeny of recursive distributional equations in Aldous and Bandyopadhyay [AB05], Bandyopadhyay [Ban02], Bandyopadhyay [Ban], Warren [War05], the local weak convergence properties Aldous and Steele [AS03], Gamarnik, Nowicki and Swirscsz [GNSa],[GNSb], Gamarnik [Gam04], and the problems of reconstruction on a tree, Mossel[Mos04], Yet, the importance of the correlation decay property for the uniqueness of Gibbs distribution was well recognized long time ago in the fundamental works by Dobrushin [Dob70] dating back to 70's. While Dobrushin's work was conducted primarily for lattices, there is a recent extension of this work by Weitz [Wei05] to more general graphs.

In this paper we establish the correlation decay property for independent sets, similar to the one considered by Kelly [Kel85] but for an arbitrary (not necessarily regular) tree with maximum degree at most 4. This property coupled with the cavity trick (2.1) almost immediately leads to a simple algorithm for computing approximately the partition function for independent sets. The corresponding algorithm for colorings is obtained by a simple extension of the Jonasson's [Jon02] uniqueness theorem for colorings.

Our explicit results for regular graphs are obtained by combining these correlation decay properties with explicit computations of marginal probabilities and a trick introduced by Mezard and Parisi [MP05], (see also Rivoire et.al [RBMM04]). The regime corresponding to our counting problem is called a *liquid phase* in these papers and the solution is obtained via replica symmetry method. Our results with respect to random regular graphs thus can be viewed as a rigorous treatment of this liquid phase solution for independent sets model.

The rest of the paper is organized as follows. In the following section we provide the necessary background and definitions. Main results and their extensions, including the extensions to random regular graphs are presented in Section 3. Proofs are derived in Sections 4,5. Due to page limitations most of the proofs are omitted and we refer the reader to the upcoming journal version of the paper.

2 Notations and basics

Throughout the paper we consider a simple graph G with the node set $V = \{v_1, \dots, v_n\}$ and edge set $E = \{e_1, \dots, e_m\}$. We also write $n = n(G) = |V|$ for the number of nodes in the graph. With some abuse of notation we will be writing $v \in G$, if node v belongs to the node set V of the graph G. For every $v \in G$, $r(v) = r(v, G)$ denotes the degree of v in G. $N(v, G)$ denotes the set of neighbors of v in G. The maximum degree and the girth (size of the smallest cycle) of G are denoted by $r = r(G) = \max_{1 \le k \le n} r(v_k)$ and $g = g(G)$ respectively. Typically, we will be considering graphs with constant r, but girth diverging to infinity as a function of n. For every positive integer t and every node v_i, we denote by $T(v_i, t)$ the depth-t neighborhood of v_i – the set of nodes reachable from v_i by paths of lengths at most t. Clearly $g > 2t$ implies that $T(v_i, t)$ is a tree for every node v_i. A set $I \subset V$ is independent (stable) if no two nodes of I share an edge. $\mathcal{I} = \mathcal{I}(G)$ denotes the set of all independent sets in G. A proper coloring $C \in \mathcal{C}(q)$ is an assignment $C : V \to \{1, \dots, q\}$ of nodes V to colors $1, 2, \dots, q$ such that no two nodes which share an edge are assigned to the same color. For every $q \in \mathbb{N}$, $\mathcal{C}(q, G) = \mathcal{C}(q)$ denotes the set of all proper colorings of the nodes of G by colors $1, 2, \dots, q$. Throughout the paper we will only consider the case $q \ge r + 1$. Then, as is well-known (and straightforward to show), the set $\mathcal{C}(q)$ is non-empty.

A classical object in statistical physics is Gibbs probability distribution on the sets $\mathcal{I}, \mathcal{C}(q)$. Fix $\lambda > 0, \lambda_j, 1 \le j \le q$ called activity parameters. The Gibbs distribution on the set $\mathcal{I}$ assigns a probability proportional to $\lambda^{|I|}$ to each independent set I:

$$\mathbb{P}(\boldsymbol{I} = I) = \frac{\lambda^{|I|}}{Z(\lambda)},$$

where $\boldsymbol{I}$ is the random (with respect to Gibbs measure) independent set, and $Z(\lambda) = Z(\lambda, G) = \sum_{I \in \mathcal{I}} \lambda^{|I|}$, the normalizing constant, is called the partition function. λ is called inverse temperature and the quantity $\log Z(\lambda)$ is also called *free energy*. In order to emphasize the underlying graph, sometimes we will denote the Gibbs measure by $\mathbb{P}_G(\cdot)$. When $\lambda = 1$, $Z(\lambda, G) = Z(1, G) = |\mathcal{I}|$ and the Gibbs distribution is simply the uniform distribution on the set of all independent sets.

There exists a way to represent the partition function $Z(\lambda, G)$ in terms of marginals of the Gibbs measure in the following sense. Let $G_0 = G$ and $G_k = G \setminus \{v_1, \dots, v_k\}, k = 1, 2, \dots, n$.

PROPOSITION 1. *The following relation holds*

$$\text{(2.1)} \qquad \frac{Z(\lambda, G_k)}{Z(\lambda, G_{k-1})} = \mathbb{P}_{G_{k-1}}(v_k \notin \boldsymbol{I}).$$

As a result,

$$\text{(2.2)} \qquad Z(\lambda, G) = \prod_{k=1}^{n} \mathbb{P}^{-1}_{G_{k-1}}(v_k \notin \boldsymbol{I}).$$

This proposition is well known and is used for Markov chain based approximation algorithms for counting. We provide the proof for completeness. For convenience we assume that a partition function of an empty graph is equal to the unity.

Proof. The proof is obtained by considering a telescoping product $Z(\lambda, G) = \prod_{k=1}^{n} \frac{Z(\lambda, G_{k-1})}{Z(\lambda, G_k)}$ and observing

$$\mathbb{P}_{G_{k-1}}(v_k \notin \boldsymbol{I}) = \frac{\sum_{I \in \mathcal{I}(G_{k-1}): v_k \notin I} \lambda^{|I|}}{Z(\lambda, G_{k-1})} = \frac{Z(\lambda, G_k)}{Z(\lambda, G_{k-1})}. \quad \blacksquare$$

For the case of coloring, the Gibbs distribution on the set $\mathcal{C}(q)$ of proper colorings is introduced similarly as

$$\mathbb{P}(\boldsymbol{C} = C) = \frac{\prod_{1 \le j \le q} \lambda_j^{|C_j|}}{Z(\lambda)},$$

where $\boldsymbol{C}$ is the (Gibbs) random coloring and $\lambda = (\lambda_1, \dots, \lambda_q)$ is a fixed vector of activity parameters, $C_j = \{v \in V : C(v) = j\}$, and $Z(\lambda) = Z(\lambda, G) = \sum_{C \in \mathcal{C}(q)} \prod_{1 \le j \le q} \lambda_j^{|C_j|}$ is again the normalizing partition function. Again the special case $\lambda_j = 1, 1 \le j \le q$ corresponds to the uniform distribution on the set $\mathcal{C}(q)$ of proper q-colorings. In this paper we focus exclusively on this special case and use notation $Z(q, G)$ or $Z(G)$ instead. We now derive an analogue of Proposition 1. For a random coloring $\boldsymbol{C}$ selected according to the Gibbs distribution and for any subset of nodes A, denote by $\boldsymbol{C}(A)$ the set of colors assigned to A. In particular, $\boldsymbol{C}(N(v_k, G_{k-1}))$ is the set of colors used by coloring $\boldsymbol{C}$ for the neighbors of the node v_k in the graph G_{k-1}. Again for convenience we assume that the number of proper q-colorings of an empty graph is equal to unity.

Proposition 2. *The following relation holds*

$$\frac{Z(G_{k-1})}{Z(G_k)} = q - \mathbb{E}_{G_k}\left[|\boldsymbol{C}(N(v_k, G_{k-1}))|\right]. \tag{2.3}$$

As a result,

$$Z(G) = \prod_{k=1}^{n}\Big[q - \mathbb{E}_{G_k}\left[|\boldsymbol{C}(N(v_k, G_{k-1}))|\right]\Big]. \tag{2.4}$$

Proof. The second part is obtained again by considering a telescoping product $Z(G) = \prod_{1\le k\le n}\frac{Z(G_{k-1})}{Z(G_k)}$. To prove the first part we observe that

$$Z(G_{k-1}) = \sum_{1\le m\le r(v_k, G_{k-1})} (q-m)\Big|\{C \in \mathcal{C}(G_k) : C(N(v_k, G_{k-1})) = m\}\Big|$$

where we simply observe that if the coloring C uses m colors for the neighbors of v_k in G_{k-1} then there are $q-m$ colors left for v_k itself. Then we divide both parts by $Z(G_k)$ and observe that

$$\sum_{m=1}^{r(v_k, G_{k-1})} m\frac{\Big|\{C \in \mathcal{C}(G_k) : C(N(v_k, G_{k-1})) = m\}\Big|}{Z(G_k)} = \mathbb{E}_{G_k}[|\boldsymbol{C}(N(v_k, G_{k-1}))|]. \quad \blacksquare$$

3 Problem formulation and results

Definition 1. *Value $\alpha > 0$ is defined to be ϵ-approximation of the log-partition function $\log Z(\lambda, G)$ if*

$$(1-\epsilon)\frac{\log Z(\lambda, G)}{n} \le \alpha \le (1+\epsilon)\frac{\log Z(\lambda, G)}{n}.$$

Given a family of graphs $\mathcal{G}$, an algorithm $\mathcal{A}$ is said to be Polynomial Approximation Scheme (PAS) for computing the log-partition function if for every n-node graph $G \in \mathcal{G}$ it produces an ϵ-approximation of $\log Z(G)$ in time which is polynomial in n.

An (infinite) family of graphs $\mathcal{G}$ is defined to have *large girth* if there exists an increasing function $f : \mathbb{N} \to \mathbb{N}$ such that $\lim_{s\to\infty} f(s) = \infty$ and for every $G \in \mathcal{G}$ with n nodes

$$g(G) \ge f(n).$$

Our first result establishes existence of PAS for computing the logarithm of the number of independent sets in graphs.

Theorem 3.1. *For every family $\mathcal{G}$ of graphs G with maximum degree $r \le 4$ and large girth, the problem of computing $\log Z(\lambda, G)$ when $\lambda = 1$ is PAS.*

We have noted in the introduction that a Markov chain based FPRAS has been established by Luby and Vigoda [LV97] for all graphs with maximum degree at most 4. We do not know whether these apparently similar restrictions are merely a coincidence or not.

Our corresponding result for counting proper colorings does not require any upper bound on the maximum degree.

Theorem 3.2. *Given a constant r, let $\mathcal{G}$ be an arbitrary family of graphs G with maximum degree r and large girth. For every constant $q \ge r+1$ the problem of computing $\log Z(q, G)$ is PAS.*

Our next results provide explicit estimates for the cardinality of the number of independent sets $\mathcal{I}$ and colorings $\mathcal{C}(q)$ in the special case of regular graphs with high girth. Let $\mathcal{G}(n, g, r)$ be the set of all r-regular graphs G with n nodes and girth at least g.

Theorem 3.3. *Suppose $\lambda < (r-1)^{r-1}/(r-2)^r$. Then $Z(\lambda, G)$ is asymptotically equal to $(x^{-\frac{r}{2}}(2-x)^{-\frac{r-2}{2}})^n$, where x is the unique solution of $x = 1/(1+\lambda x^{r-1})$. Precisely, for every $\epsilon > 0$ there exist $n_0 = n_0(\epsilon, r, \lambda)$ and $g_0 = g_0(\epsilon, r, \lambda)$ such that for all $n > n_0, g > g_0$*

$$\sup_{G\in\mathcal{G}(n,g,r)}\Big|\frac{\log Z(\lambda, G)}{n} - \log\left(x^{-\frac{r}{2}}(2-x)^{-\frac{r-2}{2}}\right)\Big| < \epsilon.$$

As a result, when $r = 2, 3, 4, 5$, $|\mathcal{I}(G)|$ is asymptotically $(1.618\ldots)^n$, $(1.545\ldots)^n$, $(1.494\ldots)^n$ and $(1.453\ldots)^n$, respectively,

Remark : One important corollary of this result is that the asymptotic value of the log-partition function is the same for every r-regular graph with large girth. Such insensitivity result cannot be obtained by the Markov Chain sampling technique.

We now state our main results for coloring. As we already mentioned, we only consider the special case $\lambda_j = 1, 1 \le j \le q$, that is the problem of counting the number of colorings. The reason for this limitation will be apparent when we discuss a recent result by Jonasson [Jon02].

Theorem 3.4. *For every $q \geq r+1$, the number of q-colorings of graphs $G \in \mathcal{G}(n,g,r)$ is asymptotically*

$$\Big[q\big(1-\frac{1}{q}\big)^{\frac{r}{2}}\Big]^n,$$

Precisely, for every $\epsilon > 0$ there exists $n_0 = n_0(\epsilon, r, q)$ and $g_0 = g_0(\epsilon, r, q)$ such that for all $n > n_0, g > g_0$

$$\sup_{G\in\mathcal{G}(n,g,r)}\Big|\frac{\log Z(q,G)}{n} - \log\Big[q\big(1-\frac{1}{q}\big)^{\frac{r}{2}}\Big]\Big| < \epsilon.$$

The following corollary is immediate from Theorem 3.4.

Corollary 1. *For every constant $\alpha \geq 1$, the number of $q = \lfloor \alpha r \rfloor + 1$ colorings of graphs $G \in \mathcal{G}(n,g,r)$ is asymptotically $(qe^{-\frac{1}{2\alpha}})^n$ as $n, r \to \infty$.*

Recently Bezakova, et.al [BSVV] obtained the following lower bound on $|\mathcal{C}(q,G)|$ in arbitrary n-node graph with maximum degree r: $|\mathcal{C}(q,G)| \geq (q - r(1-e^{-1}))^n$. Thus, when r is large and $q = \alpha r$ for some constant α, their bound becomes asymptotically $(q(1-\alpha^{-1}+(\alpha e)^{-1})^n$. It is not hard to see that the lower bound of Corollary 1 is strictly superior. For example, when $\alpha = 1$, their bound gives asymptotically $(qe^{-1})^n$ colorings, whereas, per our result, the correct asymptotic value is $(q/\sqrt{e})^n$. Of course out correct expression for the exponent comes at a cost of the large girth requirement.

3.1 Applications to random regular graphs

Random graphs are obtained by drawing a graph from some family of graphs at random according to some (typically uniform) distribution. Specifically, an r-regular n-node random graph $G_r(n)$ is obtained by selecting an r-regular graph uniformly at random from the set of all r-regular graphs on n-nodes. An important feature of such a regular graph is that the number of small cycles is small, [JŁR00]. Thus, *essentially* such graphs have a large girth and we may expect that our results for regular graphs with large girth extend to this class of graphs. It is indeed the case as we state below. The derivation of these results is very similar to the one used for the class $\mathcal{G}(n,g,r)$.

Theorem 3.5. *For every r and every $\lambda < (r-1)^{r-1}/(r-2)^r$, the partition function $Z(\lambda, G_r(n))$ of $G_r(n)$ corresponding to independent sets satisfies*

$$\frac{\log Z(\lambda, G_r(n))}{n} \to \log\big[x^{-\frac{r}{2}}(2-x)^{-\frac{r-2}{2}}\big],$$

with high probability (w.h.p.), as $n \to \infty$.

Our corresponding result for colorings is as follows.

Theorem 3.6. *For every r and every $q \geq r+1$, the partition function $Z(q, G_r(n))$ of $G_r(n)$ corresponding to the uniform distribution on proper q-colorings satisfies*

$$\frac{\log Z(q, G_r(n))}{n} \to \log\Big[q\big(1-\frac{1}{q}\big)^{\frac{r}{2}}\Big].$$

w.h.p. as $n \to \infty$.

4 Counting independent sets

The key method for obtaining the results in this paper is establishing a very strong form of correlation decay, appropriately defined. Correlation decay is one of the key concepts in statistical physics which has been used to established the uniqueness of Gibbs distribution on infinite graphs (on finite graphs Gibbs distribution is unique by definition). These questions of uniqueness and correlation decay have been considered primarily in on regular trees. Here we reconstruct some of these results and extend them to non-regular trees. A strong form of correlation decay which we will establish will then be used to project our results to arbitrary graphs with large girth (and additional restrictions dictated by a particular context).

4.1 Independent sets on trees and correlation decay Let T be an arbitrary tree with depth at most t. That is the distance from the root (denoted v_0) to any other node $v \in T$ is at most t. Denote by $B(T)$ the boundary of the tree – the set of nodes with distance exactly t from the root. Any function $b : B(T) \to \{0,1\}$ is called a boundary condition b. When $B(T)$ is empty the boundary condition is not defined. We think of boundary condition as conditioning on which nodes on the boundary belong to an independent set (corresponding value is 1) and which do not (value is zero). In particular, for any boundary condition b, we denote by $\mathbb{P}(v_0 \in \boldsymbol{I}|b)$ the probability of the event "v_0 belongs to the random independent set $\boldsymbol{I}$", conditioned on the event $\{v \in B(T) : v \in \boldsymbol{I}\} = \{v \in B(T) : b(v) = 1\}$, with respect to the Gibbs measure. Denote by $\mathcal{B}(T)$ the set of all boundary conditions b on T, and denote by $\mathcal{T}(t,r)$ the set of all trees with maximum degree at most r and depth at most t.

Our first result establishes the key correlation decay property of Gibbs distributions of independent sets on trees with maximum degree at most 4.

Proposition 3. *The following bounds holds for every $t \geq 2$, $T \in \mathcal{T}(t,4), b, b_1, b_2 \in \mathcal{B}(T)$*

$$\frac{1}{2} \leq \mathbb{P}(v_0 \notin \boldsymbol{I}|b) \leq \frac{8}{9}. \tag{4.5}$$

and

$$\Big|\mathbb{P}(v_0 \notin \boldsymbol{I}|b_1) - \mathbb{P}(v_0 \notin \boldsymbol{I}|b_2)\Big| \le (.9)^{t-2}. \tag{4.6}$$

where $\mathbb{P}(\cdot)$ *is with respect to the Gibbs distribution with* $\lambda = 1$.

Moreover, given λ *satisfying* $\lambda < (r-1)^{r-1}/(r-2)^r$, *let* x *be the unique non-negative solution of the equation* $x = 1/(1+\lambda x^{r-1})$. *Suppose all the nodes of* T *except for leaves and the root have degree* r, *and suppose the root has degree* $r-1$. *Then for all* $b \in \mathcal{B}(T)$

$$\big|\mathbb{P}(v_0 \notin \boldsymbol{I}|b) - x\big| \le \alpha^t, \tag{4.7}$$

for some constant $\alpha = \alpha(\lambda) < 1$. *If, on the other hand, all the nodes except for leaves, have degree* r *(including the root), then*

$$\big|\mathbb{P}(v_0 \notin \boldsymbol{I}|b) - \frac{1}{2-x}\big| \le \alpha^t, \tag{4.8}$$

for the same constant α.

Remark : The second part of the proposition is a known result established first in Kelly [Kel85]. and thus we simply refer to Kelly's work for the proof. See also [BW04] (where w corresponds to $1/x - 1$), and Bandyopadhyay [Ban] where the latter work is concerned with the extension of Kelly's result to general Galton-Watson type random trees. The constant $\alpha(\lambda)$ approaches unity as λ approaches $(r-1)^{r-1}/(r-2)^r$ and can expressed explicitly, but this is not required for our paper.

Proof. We fix a tree $T \in \mathcal{T}(t,r)$ and activity λ. Denote by $v_1,\ldots,v_k, k \le r$ the neighbors $N(v_0,T)$ of the root. This includes the possibility $k=0$ (the tree consists of only node v_0). For every node $v \in T$, $T(v)$ denotes the subtree rooted at v not containing v_0, and $b(T(v))$ denotes the natural restriction of a boundary condition $b \in \mathcal{B}(T)$ to $T(v)$. For every node v, let $T(v|b)$ be the tree obtained by deleting the leaves $v' \in T(v)$ which have value $b(v') = 1$ as well as their parent nodes. Let $J = I \cap T(v|b)$. It is immediate that for every independent set $I \subset T$, its Gibbs probability with boundary condition b is

$$\mathbb{P}_T(\boldsymbol{I} = I | I \cap B(T) = b) = \mathbb{P}_{T(v|b)}(\boldsymbol{I} = J) = \frac{\lambda^{|J|}}{\sum_{J' \in \mathcal{I}(T(v|b))} \lambda^{|J'|}},$$

Using convention $\prod_{1\le j\le k} = 1$ when $k=0$, we obtain

$$\begin{aligned} Z(\lambda, T(v_0|b)) &= \sum_{I \in \mathcal{I}(T(v_0|b))} \lambda^{|I|} \\ &= \prod_{1\le j\le k}\Big(\sum_{I\in\mathcal{I}(T(v_j|b))}\lambda^{|I|}\Big) \\ &\quad + \lambda \prod_{1\le j\le k}\Big(\sum_{I\in\mathcal{I}(T(v_j|b)), v_j\notin I}\lambda^{|I|}\Big) \end{aligned}$$

We recognize that

$$\frac{\prod_{1\le j\le k}\Big(\sum_{I\in\mathcal{I}(T(v_j|b))}\lambda^{|I|}\Big)}{Z(\lambda,T(v_0|b))} = \frac{\prod_{1\le j\le k} Z(\lambda, T(v_j|b))}{Z(\lambda, T(v_0|b))} = \mathbb{P}_{T(v_0)}(v_0 \notin \boldsymbol{I}|b)$$

Using the previous expression for $Z(\lambda, T(v_0|b))$, we obtain

$$\mathbb{P}_{T(v_0)}(v_0 \notin \boldsymbol{I}|b) = \frac{1}{1+\lambda\prod_{1\le j\le k}\mathbb{P}_{T(v_j)}(v_j \notin \boldsymbol{I}|b)}. \tag{4.9}$$

Note, that similar recursion applies to any node v substituting the root v_0 by replacing T with $T(v)$. Specifically, take any node v which is a parent of a leaf in level t in a main tree T, if any exist. That is v is located on level $t-1$. It has $r(v)-1$ children which we denote by $v_1,\ldots,v_{r(v)-1}$ its children. For every child $v_j, j \le r(v)-1$ (if there are any) the value $\mathbb{P}(v_j \notin \boldsymbol{I}|b)$ is either zero or one depending on whether $b(v_j) = 0$ or $= 1$. The recursive equation (4.9) implies that $\mathbb{P}_{T(v)}(v \notin \boldsymbol{I}|b) \in [(1+\lambda)^{-1}, 1]$.

Now, suppose that v is any node on level $t-2$ and suppose it has $r(v)-1$ children. Then applying the same recursion and the previously obtained bounds, we get

$$\frac{1}{1+\lambda} \le \mathbb{P}(v \notin \boldsymbol{I}|b) \le \frac{1}{1+\lambda(1+\lambda)^{-r(v)+1}} \le \frac{1}{1+\lambda(1+\lambda)^{-r+1}}.$$

For every node v in level $t-2$ define $a(v) = 1/(1+\lambda)$ and $c(v) = 1/(1+\lambda(1+\lambda)^{-r+1})$ and now we obtain bounds on probability $\mathbb{P}(v \notin \boldsymbol{I}|b)$ nodes at lower levels. Given a node v in level $\tau \le t-2$, suppose $\mathbb{P}(v \notin \boldsymbol{I}|b)$ belongs to an interval $[a(v), c(v)]$. Then for every node v with children nodes $v_1,\ldots,v_{r(v)-1}$ we obtain

$$a(v) = \frac{1}{1+\lambda\prod_{1\le j\le r(v)-1} c(v_j)} \le \mathbb{P}(v \notin \boldsymbol{I}|b) \tag{4.10}$$

$$\le \frac{1}{1+\lambda\prod_{1\le j\le r(v)-1} a(v_j)} = c(v). \tag{4.11}$$

Also, inductively assuming $a(v_j) \geq 1/(1+\lambda), c(v_j) \leq 1/(1+\lambda(1+\lambda)^{-r+1}$, we obtain by the same argument as above that the same bounds hold for $a(v), c(v)$ for all the node v in levels up to $t-2$:

$$\text{(4.12)} \qquad \frac{1}{1+\lambda} \leq a(v) \leq c(v) \leq \frac{1}{1+\lambda(1+\lambda)^{-r+1}}.$$

We note that these bounds only depend on the tree T but not the boundary condition b. We now show that , the length of the bounding interval $c(v) - a(v)$ is geometrically decreasing in as a function of the level of v in our special case of interest.

LEMMA 4.1. *Suppose $r = 4, \lambda = 1$. Then for every node $v \in T$ in level τ, $c(v) - a(v) \leq (.9)^{t-2-\tau}$.*

Proof. The proof proceeds by reverse induction in τ starting with $\tau = t-2$. It involves considering a function $f : [(1+\lambda)^{-1}, (1+\lambda(1+\lambda)^{-r+1})^{-1}]^k \to \mathbb{R}$ given by $f(z) = f(z_1, \ldots, z_k) = (1+\lambda\prod_{1\leq j\leq k} z_j)^{-1}$ and application of the Mean Value Theorem. We omit details in the interest of space.

Application of the lemma to the root node v_0 yields, $c(v_0) - a(v_0) \leq (.9)^{t-2}$. Combining this with (4.11) applied to v_0 gives for every two boundary conditions b_1, b_2

$$\Big|\mathbb{P}(v_0 \notin \boldsymbol{I}|b_1) - \mathbb{P}(v_0 \notin \boldsymbol{I}|b_2)\Big| \leq c(v_0) - a(v_0) \leq (.9)^{t-2}.$$

This establishes (4.6) and completes the proof the first part of the proposition.

The second part of the proposition is the result already established by Kelly [Kel85] and we simply refer to his paper. ■

4.2 Algorithm and the proof of Theorem 3.1

Proposition 3 establishes the key correlation decay property for independent sets for trees with maximum degree at most 4. It shows that the marginal Gibbs probability at the root is asymptotically independent from the boundary. Equipped with this result and Proposition 1, we propose the following algorithm for estimating the number of independent sets of a given graph G.

Algorithm CountIND

`INPUT: A graph G with a node set` $v_1, \ldots, v_n$ `and parameter` $\epsilon > 0$.
`BEGIN`
`1. Compute the girth` $g(G)$. `If` $(.9)^{\frac{g(G)}{2}-2} \geq \epsilon$ `compute` $\mathcal{I}(G)$ `by exhaustive enumeration. Otherwise`
`2. Set` $G' = G$, $Z = 1$, $t = g(G)/2$.
`3. Find any node` $v \in G'$ `and identify its depth`$-t$ `neighborhood` $T(v)$.
`4. Perform subroutine CountingTREE on` $T(v)$ `which results in some value` $p(v)$. `Set` Z `equal to` $Zp^{-1}(v)$.
`5. Set` $G' = G' \setminus \{v\}$ `and go to step 3.`
`END`
`OUTPUT:` Z.

Subroutine CountingTREE

`INPUT: A tree` T `with an identified root` v `and depth` t.
`BEGIN`
`1. Identify the nodes` u `in level` t `(if any exist) and set` $p(u) = 1/2$.
`FOR` $l = t-1, t-2, \ldots, 0$
`Identify a node` u `in level` l `(if any exist). If` u `has no children, set` $p(u) = 1/2$. `Otherwise set` $p(u) = 1/(1+\prod p(u_i))$, `where the product runs over children` u_i `of` u `in level` $l+1$ `and the values` $p(u_i)$ `were obtained in an earlier step.`
`END`
`OUTPUT:` $p(v)$.

Proof. Proof of Theorem 3.1. We claim that the algorithm `CountIND` provides PAS. Fix a family of graphs $\mathcal{G}$ with maximum degree $r \leq 4$ and large girth, a graph $G \in \mathcal{G}$ and $\epsilon > 0$. The algorithm first checks whether $g(G) > 4 + 2\log(1/\epsilon)/\log(10/9)$. By definition there exists a finite number of graphs in $\mathcal{G}$ with girth $\leq 4 + 2\log(1/\epsilon)/\log(10/9)$ and their corresponding values of $\mathcal{I}$ can be found in constant time, where the constant depends on ϵ and the growth rate f of girth.

Otherwise the girth satisfies $(.9)^{\frac{g(G)}{2}-2} < \epsilon$ and in the remaining n steps of the algorithm the Gibbs marginal probability $\mathbb{P}(v_k \in \boldsymbol{I})$ is computed with respect to the depth $t = g(G)/2$ neighborhood $T(v_k)$ of the node v_k with respect to the graph G_{k-1}. By selection of t, $T(v_k)$ is a tree (the girth of each subgraph G_{k-1} is trivially at least $g(G)$). The rest of the proof is obtained by taking the difference between the marginal probabilities with respect to these trees with some boundary conditions and then integrating over these boundary conditions. The main part of the argument is using Proposition 3. We omit details in the interest of space. ■

4.3 Regular graphs and proof of Theorem 3.3

In this subsection we obtain explicit asymptotics for the number of independent sets in regular graphs. Theorem 3.1 provides a way in principle for computing number of independent sets in regular graph. The problem is, however, in the fact that the cavity step expressed in (2.1) destroys regularity. The help comes from a trick invented by Mezard and Parisi [MP05] introduced in the context of random regular graph. Given an n-node r-regular G fix any two nodes v_1, v_2 which have non-intersecting neighbors and denote their non-overlapping neighbor sets by $v_{11}, \dots, v_{1r}$ and $v_{21}, \dots, v_{2r}$, respectively. Consider a modified graph G^o obtained by from G by deleting v_1, v_2 and connecting v_{1j} to $v_{2j}, j = 1, \dots, r$ by an edge. The resulting graph is r-regular again. We call this operation "rewire".

The main question is whether we can relate the partition functions of the original and modified graphs and whether the resulting graph still has a sufficiently large girth, provided the original one does. The first issue has been addressed in [MP05] and[RBMM04] and is essentially a simple combination of type (2.1) arguments. The second issue was not addressed in [MP05],[RBMM04] in a rigorous way.

We begin by addressing the second issue first.

LEMMA 4.2. *Given an n-node r-regular graph G, consider any integer $4 \le g \le g(G)$. The operation rewire can be performed for at least $(n/2) - (2g+1)r^{2g}$ steps on pairs of nodes which are at least $2g+1$ distance apart. In every step the resulting graph is r-regular with girth at least g.*

Proof. The proof is based on a straightforward combinatorial argument. We omit the details.

We now turn to the second problem of estimating the relative change of the partition function after applying the rewire operation. This relative change is called *energy shift* in [RBMM04]. First we provide an elementary analogue of (2.1).

LEMMA 4.3. *Given an r-regular graph G, given $\lambda > 0$ and graph G^o obtained from G by rewiring on nodes $v_1, v_2 \in G$, the following relation holds*

$$\frac{Z(\lambda, G^o)}{Z(\lambda, G)} = \mathbb{P}_G(v_1, v_2 \notin \boldsymbol{I}) \times$$
$$\times \mathbb{P}_{G \setminus \{v_1, v_2\}}(\wedge_{1 \le j \le r}(v_{1j} \notin \boldsymbol{I} \vee v_{2j} \notin \boldsymbol{I}))$$

where $v_{ij}, j = 1, \dots, r$ is the set of neighbors of $v_i, i = 1, 2$ in G.

Proof. The proof is almost identical to the one of Proposition 1. We skip details. ■

We now obtain a very simple limiting expression for the probability in Lemma 4.3.

LEMMA 4.4. *Given $r \in \mathbb{N}, \lambda < (r-1)^{r-1}/(r-2)^r$ and $\epsilon > 0$, there exists a sufficiently large constant $g = g(r, \epsilon, \lambda)$ such that for every graph G with girth $g(G) > g$, and for every pair of nodes $v_1, v_2 \in G$ at distance at least $2g+1$*

$$\left|\mathbb{P}_G((v_1, v_2 \notin \boldsymbol{I})) - \frac{1}{(2-x)^2}\right| < \epsilon, \tag{4.13}$$

and

$$\left|\mathbb{P}_{G \setminus \{v_1, v_2\}}\big(\wedge_{1 \le j \le r} (v_{1j} \notin \boldsymbol{I} \vee v_{2j} \notin \boldsymbol{I})\big) - (2x - x^2)^r\right| < \epsilon, \tag{4.14}$$

where $v_{ij}, j = 1, \dots, r$ is the set of neighbors of v_i in G, $i = 1, 2$, and x is the unique solution of $x = 1/(1 + \lambda x^{r-1})$.

Proof. The proof consists of several steps, each ideologically very similar to the one for Theorem 3.1 and thus details are omitted.

Proof. Proof of Theorem 3.3. The proof is obtained by combining the results of Lemmas 4.2,4.3,4.4. We show that at every step of the rewire operation, the approximate values given in Lemmas 4.3 and 4.4 hold. Then we use Lemma 4.2 to show that the rewire operation can be performed for $n - O(1)$ steps. The rest of the details of the proof are omitted. ■

5 Counting Colorings

5.1 Coloring of trees and correlation decay

We use the definitions and notations of Subsection 4.1: $T, B(T), \mathcal{B}(T)$ denote respectively an arbitrary depth-t tree with maximum degree at most r, the boundary of the tree and the set of boundary conditions. The latter, however, is defined as the set of functions $b : B(T) \to \{1, 2, \dots, q\}$ mapping nodes to colors. The root of this tree is v_0. Similarly to the case of independent set, we use notation $\mathbb{P}(\boldsymbol{C}(v) = j|b)$ to indicate probability that the random coloring $\boldsymbol{C}$ assigns color j to the node $v \in T$, subject to the boundary condition b, where probability is with respect to the Gibbs measure, (in this case uniform distribution) on the set of all proper colorings.

We establish an analogue of Proposition 3, but in this case we use the following recent result by Jonasson [Jon02]. This result was used to establish uniqueness of Gibbs measures for coloring on infinite trees, but the main underlying result is a very strong form of correlation decay.

THEOREM 5.1. (**Jonasson [Jon02].**) *Suppose $q \ge r + 1$. There exists a computable value $\beta = \beta(r) < 1$ such that for every r-regular tree T with depth t*

$$\sup_{b \in \mathcal{B}(T)} \left|\mathbb{P}(\boldsymbol{C}(v_0) = j|b) - \frac{1}{q}\right| \le \beta^t,$$

for every $j = 1, 2, \ldots, q$.

Note that the decay constant β does not even depend on q provided that $q \geq r+1$. The analysis of the proof in [Jon02] reveals that the same result holds for non-regular trees as well.

Corollary 2. *The result of Theorem 5.1 holds when* T *is an arbitrary depth-t tree with maximum degree* r.

5.2 Algorithm and the proof of Theorem 3.2

We propose the following algorithm for estimating the number of q-colorings of a given graph G.

Algorithm CountCOLOR

INPUT: A graph G with maximum degree r such that $q \geq r+1$, a node set $v_1, \ldots, v_n$, and a parameter $\epsilon > 0$.

BEGIN

1. Compute the girth $g(G)$. If $\beta^{\frac{g(G)}{2}-2} \geq \epsilon$ compute $\mathcal{C}(G)$ by exhaustive enumeration. Otherwise
2. Set $G' = G$, $Z = 1$, $t = g(G)/2$.
3. Find any node $v \in G'$ and its degree $r' = r(v, G) \leq r$. Set Z equal to $Z[q(1-\frac{1}{q})^{r'}]$.
4. Set $G' = G' \setminus \{v\}$ and go to step 2.

END

OUTPUT: Z.

Proof. Proof of Theorem 3.2. The proof is very similar to the one of Theorem 3.1. We omit details in the interest of space. ■

5.3 Regular graphs and proof of Theorem 3.4

Our main tool is again operation rewire performed on regular graphs with large girth. Given an arbitrary graph G and nodes $v_1, v_2 \in G$ such that v_1 and v_2 are not neighbors, and they do not have a common neighbor, let G^o be obtained from G by rewiring on v_1, v_2. Proposition 2 already relates the partition function of G to the one of $G \setminus \{v_1, v_2\}$. We now relate it to the one of G^o. Let $G' = G \setminus \{v_1, v_2\}$. That is G' is G^o before the pairs v_{1j}, v_{2j} are connected. Consider the random uniform q-coloring $\boldsymbol{C}$ in G'. The lemma below does not rely on assumptions of regularity or the girth size of the underlying graph G.

Lemma 5.1. *The following relation holds*

$$\frac{Z(G)}{Z(G^o)} = \frac{\mathbb{E}_{G'}\Big[\big(q - |\boldsymbol{C}(N(v_1,G))|\big)\big(q - |\boldsymbol{C}(N(v_2,G))|\big)\Big]}{\mathbb{P}_{G'}(\boldsymbol{C}(v_{1j}) \neq \boldsymbol{C}(v_{2j}),\ 1 \leq j \leq r)},$$

where $v_{ij}, j = 1, \ldots, r$ *is the set of neighbors of* $v_i, i = 1, 2$ *in* G.

Proof. Using the same argument as in Proposition 2 we obtain that

$$\frac{Z(G)}{Z(G')} = \mathbb{E}_{G'}\Big[\big(q - |\boldsymbol{C}(N(v_1,G))|\big)\big(q - |\boldsymbol{C}(N(v_2,G))|\big)\Big].$$

On the other hand $\frac{Z(G_0)}{Z(G')}$ is the probability that a randomly selected coloring in G' assigns different colors to each pair $v_{1j}, v_{2j}, j = 1, 2, \ldots, r$. Combining, we obtain the result. ■

The following lemma is an analogue of Lemma 4.4.

Lemma 5.2. *Given* $r \in \mathbb{N}$, $q \geq r+1$ $\epsilon > 0$, *there exists a sufficiently large constant* $g = g(r, \epsilon)$ *such that for every* r*-regular graph* G *with girth* $g(G) > g$, *for every pair of nodes* $v_1, v_2 \in G$ *at distance at least* $2g + 1$

$$\Big|\mathbb{E}_{G'}\Big[\big(q - |\boldsymbol{C}(N(v_1,G))|\big)\big(q - |\boldsymbol{C}(N(v_2,G))|\big)\Big] -$$

(5.15)

$$- q^2(1-\frac{1}{q})^{2r}\Big| < \epsilon.$$

(5.16)

$$\Big|\mathbb{P}_{G'}(\boldsymbol{C}(v_{1j}) \neq \boldsymbol{C}(v_{2j}),\ 1 \leq j \leq r) - (\frac{q-1}{q})^r\Big| < \epsilon.$$

Proof. The proof is very similar to the one of Lemma 4.4 and is omitted.

Proof. Proof of Theorem 3.4. The proof follows the same steps as the proof of Theorem 3.3. The results of Theorem 5.1 and Lemmas 4.2, 5.1, 5.2 are combined to obtained the limiting expression after the cancelation of $(\frac{q-1}{q})^r$. ■

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