

Improved Mixing Condition on the Grid for Counting and Sampling Independent Sets

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Abstract— The hard-core model has received much attention in the past couple of decades as a lattice gas model with hard constraints in statistical physics, a multicast model of calls in communication networks, and as a weighted independent set problem in combinatorics, probability and theoretical computer science.

In this model, each independent set I in a graph G is weighted proportionally to $\lambda^{|I|}$, for a positive real parameter λ . For large λ , computing the partition function (namely, the normalizing constant which makes the weighting a probability distribution on a finite graph) on graphs of maximum degree $\Delta \geq 3$, is a well known computationally challenging problem. More concretely, let $\lambda_c(\mathbb{T}_\Delta)$ denote the critical value for the so-called uniqueness threshold of the hard-core model on the infinite Δ -regular tree; recent breakthrough results of Dror Weitz (2006) and Allan Sly (2010) have identified $\lambda_c(\mathbb{T}_\Delta)$ as a threshold where the hardness of estimating the above partition function undergoes a computational transition.

We focus on the well-studied particular case of the square lattice \mathbb{Z}^2 , and provide a new lower bound for the uniqueness threshold, in particular taking it well above $\lambda_c(\mathbb{T}_4)$. Our technique refines and builds on the tree of self-avoiding walks approach of Weitz, resulting in a new technical sufficient criterion (of wider applicability) for establishing strong spatial mixing (and hence uniqueness) for the hard-core model. Our new criterion achieves better bounds on strong spatial mixing when the graph has extra structure, improving upon what can be achieved by just using the maximum degree. Applying our technique to \mathbb{Z}^2 we prove that strong spatial mixing holds for all $\lambda < 2.3882$, improving upon the work of Weitz that held for $\lambda < 27/16 = 1.6875$. Our results imply a fully-polynomial *deterministic* approximation algorithm for estimating the partition function, as well as rapid mixing of the associated Glauber dynamics to sample from the hard-core distribution.

1. INTRODUCTION

In this paper we study phase transitions for sampling weighted independent sets (weighted by an activity $\lambda > 0$) of the 2-dimensional integer lattice \mathbb{Z}^2 . In statistical physics terminology, we study the hard-core lattice gas model ([6], [13]), which is a simple model of a gas whose particles have non-negligible size (thus preventing them from occupying

neighboring sites), with activity $\lambda \in \mathbb{R}_+$ corresponding to the so-called fugacity of the gas. More formally, for a finite graph $G = (V, E)$, let $\Omega = \Omega(G)$ denote the set of independent sets of G . Given an independent set $\sigma \in \Omega$, its weight is defined as $w(\sigma) = \lambda^{|\sigma|}$ and $v \in V$ is said to be occupied under σ if $v \in \sigma$. The associated Gibbs (or Boltzmann) distribution $\mu = \mu_{G,\lambda}$ is defined on Ω as $\mu(\sigma) = w(\sigma)/Z$, where $Z = Z(G, \lambda) = \sum_{\eta \in \Omega} w(\eta)$ is commonly referred to as the partition function.

Recall that Valiant [32] showed that *exactly computing* the number of independent sets is #P-complete, even when restricted to 3-regular graphs (see Greenhill [16]). Hence, we focus our attention on approximation algorithms for estimating the number, or more generally, the partition function. It is well known [17] that the problem of approximating the partition function Z and that of sampling from a distribution that is close to the Gibbs distribution μ , are polynomial-time reducible to each other (see also [30]).

The fundamental notion of a phase transition for a statistical mechanics model on an infinite graph addresses the critical point at which the model starts to exhibit a certain long-range dependence, as a system parameter is varied. In particular, the so-called critical inverse temperature β_c for the Ising or the Potts model, and the critical activity λ_c for the hard-core lattice gas model, are prime examples where the system undergoes a transition from uniqueness to multiplicity of the infinite-volume Gibbs measures.

Phase transition in the hard-core model is also intimately related to the computational complexity of estimating the partition function Z . Recently, a remarkable connection was established between the computational complexity of approximating the partition function for graphs of maximum degree Δ and the phase transition $\lambda_c(\mathbb{T}_\Delta)$ for the infinite regular tree \mathbb{T}_Δ of degree Δ . On the positive side, Weitz [33] showed a deterministic fully-polynomial time approximation algorithm (FPAS) for approximating the partition function for any graph with maximum degree Δ , when $\lambda < \lambda_c(\mathbb{T}_\Delta)$ and Δ is constant. On the other side, Sly [29] recently showed that for every $\Delta \geq 3$, it is NP-hard (unless NP=RP) to approximate the partition function for graphs of maximum degree Δ , when $\lambda_c(\mathbb{T}_\Delta) < \lambda < \lambda_c(\mathbb{T}_\Delta) + \epsilon_\Delta$, for some function $\epsilon_\Delta > 0$. More recently, Galanis et al. [12] improved the range of λ in Sly's inapproximability result, extending it to all $\lambda > \lambda_c(\mathbb{T}_\Delta)$ for the cases $\Delta = 3$ and $\Delta \geq 6$.

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1.1. Prior history and current work

Our work builds upon Weitz’s work to get improved results for specific graphs of interest. We focus our attention on what is arguably the simplest, not yet well-understood, case of interest namely the square grid, or the 2-dimensional integer lattice \mathbb{Z}^2 . Empirical evidence suggests that the critical point $\lambda_c(\mathbb{Z}^2) \approx 3.796$ [13], [3], [25], but rigorous results are significantly far from this conjectured point. The possibility of there being multiple such λ_c is not ruled out, although no one believes that this is the case.

From below, van den Berg and Steif [6] used a disagreement percolation argument to prove $\lambda_c(\mathbb{Z}^2) > \frac{p_c}{1-p_c}$ where p_c is the critical probability for site percolation on \mathbb{Z}^2 . Applying the best known lower bound on $p_c > 0.556$ for \mathbb{Z}^2 by van den Berg and Ermakov [5] implies $\lambda_c(\mathbb{Z}^2) > 1.252\dots$. Prior to that work, an alternative approach aimed at establishing the Dobrushin-Shlosman criterion [10], yielded, via computer-assisted proofs, $\lambda_c(\mathbb{Z}^2) > 1.185$ by Radulescu and Styer [27], and $\lambda_c(\mathbb{Z}^2) > 1.508$ by Radulescu [26].

These results were improved upon by Weitz [33] who showed that $\lambda_c(\mathbb{Z}^2) \geq \lambda_c(\mathbb{T}_4) = 27/16 = 1.6875$, where \mathbb{T}_Δ is the infinite, complete, regular tree of degree Δ . For the upper bound, a classical Peierls’ type argument implies $\lambda_c(\mathbb{Z}^2) = O(1)$ [9]. (A related result of Randall [28] showing slow mixing of the Glauber dynamics for $\lambda > 8.066$ gives hope for a better upper bound on $\lambda_c(\mathbb{Z}^2)$.) The regular tree \mathbb{T}_Δ is one of the only examples (that we know of) where the critical point is known exactly, and in this case, Kelly [18] showed that $\lambda_c(\mathbb{T}_\Delta) = (\Delta - 1)^{\Delta-1}/(\Delta - 2)^\Delta$.

In this work we present a new general approach which, for the case of the hard-core model on \mathbb{Z}^2 , improves the lower bound to $\lambda_c(\mathbb{Z}^2) > 2.3882$. There are various algorithmic implications for finite subgraphs of the \mathbb{Z}^2 when $\lambda < 2.3882$. Our results imply that Weitz’s deterministic FPAS is also valid on subgraphs of \mathbb{Z}^2 for the same range of λ . Thanks to the existing literature on general spin systems ([21], [22], [8], [11]), our results also imply that the Glauber dynamics has $O(n \log n)$ mixing time for any finite subregion $G = (V, E)$ of \mathbb{Z}^2 when $\lambda < 2.3882$, where $n = |V|$. Recall that the Glauber dynamics is a simple Markov chain that updates the configuration at a randomly chosen vertex in each step, see [19] for an introduction to the Glauber dynamics. The stationary distribution of this chain is the Gibbs distribution. Hence, it is of interest as an algorithmic technique to randomly sample from the Gibbs distribution, and also as a model of how physical systems reach equilibrium. The mixing time is the number of steps (from the worst initial configuration) until the distribution is guaranteed to be within variation distance $\leq 1/4$ of the stationary distribution.

As in Weitz’s work, our approach can be used for other 2-spin systems, such as the Ising model (see the full version of this paper [36] for more details). As will be evident from

the following high-level idea of our approach, it can be applied to other graphs of interest. Our work also provides an arguably simpler way to derive the main technical result of Weitz showing that any graph with maximum degree Δ has strong spatial mixing (SSM) when $\lambda < \lambda_c(\mathbb{T}_\Delta)$.

To underline the difficulty in estimating bounds on λ_c , we remark that the *existence* of a (unique) critical activity λ_c remains conjectural and an open problem for \mathbb{Z}^d , for $d \geq 2$. In contrast, for the Ising model, the critical inverse temperature $\beta_c(\mathbb{Z}^2)$ has been known since 1944 [23]; interestingly, the corresponding critical point for the q -state Potts model (for $q \geq 2$) has only recently been established (by Beffara and Duminil-Copin [4]) to be $\beta_c(q) = \log(1 + \sqrt{q})$, settling a long-standing open problem. The lack of monotonicity in λ in the hard-core model poses a serious challenge in establishing such a sharp result for this model. In fact, Brightwell et al. [7] showed that in general such a monotonicity need not hold, by providing an example with a non-regular tree.

2. TECHNICAL PRELIMINARIES AND PROOF APPROACH

Before presenting our approach, it is useful to review briefly the uniqueness/non-uniqueness phase transition, and introduce associated notions of decay of spatial correlation, known as weak and strong spatial mixing properties. Much of the below discussion is simplified for the case of the hard-core model on \mathbb{Z}^2 , wherein one utilizes certain induced monotonicity (given by the bipartite property) in the model and the amenability of the graph.

2.1. Uniqueness, Weak and Strong Spatial Mixing

Let B_L denote the finite graph corresponding to a box of side-length $2L + 1$ centered around the origin in \mathbb{Z}^2 . Thus, $B_L = (V, E)$, where $V = \{(i, j) \in \mathbb{Z}^2 : -2L - 1 \leq i, j \leq 2L + 1\}$ with edges between pairs of vertices at L_1 distance (or Manhattan distance) equal to one. Since this is a bipartite graph, we may fix one such partition $V = \text{even} \cup \text{odd}$ – for example, it is standard to consider the set of vertices at an even distance from the origin as the even set. The boundary of B_L are those vertices $v = (v_1, v_2) \in V$ where $|v_i| = 2L + 1$ for $i = 1$ or $i = 2$. The hard-core model on bipartite graphs is a monotone system (e.g., see [11]), which for the current discussion implies that we only have to consider two assignments to the boundary: all even vertices or all odd vertices on the boundary are occupied. Let $\alpha_{L,r}^{\text{even}}$ ($\alpha_{L,r}^{\text{odd}}$) denote the marginal probability that the origin r is unoccupied given the even (odd, respectively) boundary. Then to establish uniqueness of the Gibbs measures, we need that:

$$\lim_{L \rightarrow \infty} |\alpha_{L,r}^{\text{even}} - \alpha_{L,r}^{\text{odd}}| = 0.$$

We are interested in the critical point λ_c for the transition between uniqueness and non-uniqueness. A standard way to establish uniqueness is by proving one of the spatial mixing properties introduced next.

Let $G = (V, E)$ be a (finite) graph. For $S \subset V$, a configuration ρ on S specifies a subset of S as occupied and the remainder as unoccupied. Let $\mu^\rho = \mu_G^\rho$ denote the Gibbs distribution conditional on configuration ρ to S . For $v \in V$, let $\alpha_v^\rho = \alpha_{G,v}^\rho$ denote the marginal probability that v is unoccupied in μ^ρ .

The first spatial mixing property is *Weak Spatial Mixing (WSM)*. Here we consider a pair of boundary configurations on a subset S and consider the ‘‘influence’’ on the marginal probability that a vertex v is unoccupied. WSM says that the influence on v decays exponentially in the distance of S from v .

Definition 1 (Weak Spatial Mixing): For the hard-core model at activity λ , for finite graph $G = (V, E)$, WSM holds with rate $\gamma \in (0, 1)$ if for every $v \in V$, every $S \subset V$, and every two configurations ρ, η on S ,

$$|\alpha_v^\rho - \alpha_v^\eta| \leq \gamma^{\text{dist}(v, S)}$$

where $\text{dist}(v, S)$ is the graph distance (i.e., length of the shortest path) between v and (the nearest point in) the subset S .

The second property of interest is *Strong Spatial Mixing (SSM)*. The intuition is that if a pair of boundary configurations on a subset S agree at some vertices in S then those vertices ‘‘encourage’’ v to agree. Therefore, SSM says that the influence on v decays exponentially in the distance of v from the subset of vertices where the pair of configurations differ.

Definition 2 (Strong Spatial Mixing): For the hard-core model at activity λ , for finite graph $G = (V, E)$, SSM holds with rate $\gamma \in (0, 1)$ if for every $v \in V$, every $S \subset V$, every $S' \subset S$, and every two configurations ρ, η on S where $\rho(S \setminus S') = \eta(S \setminus S')$,

$$|\alpha_v^\rho - \alpha_v^\eta| \leq \gamma^{\text{dist}(v, S')}.$$

Note that since $\text{dist}(v, T) \leq \text{dist}(v, T \setminus S)$, SSM implies WSM for the same rate. Moreover, it is a standard fact that such an exponential decay in finite boxes (say), in \mathbb{Z}^d , implies uniqueness of the corresponding infinite volume Gibbs measure on \mathbb{Z}^d , see Georgii [14] for an introduction to the theory of infinite-volume Gibbs measures. We can specialize the above notions of WSM and SSM to a particular vertex v , in which case we say that WSM or SSM holds *at* v . If the graph is a rooted tree, we will always assume that the notions of WSM and SSM are considered at the root.

For the hard-core model on a graph $G = (V, E)$, for a subset of vertices S and a fixed configuration ρ on S , it is equivalent to consider the subgraph G' which we obtain for each $v \in S$ that is fixed to be unoccupied we remove v from G , and for each $v \in S$ that is fixed to be occupied we remove v and its neighbors $N(v)$ from G . In this way we obtain the following observation which will be useful for proving SSM holds.

Observation 1: For a graph $G = (V, E)$ and $v \in V$, SSM holds in G at vertex v iff WSM holds for all subgraphs G' (of G) at vertex v . To be precise, by subgraphs we mean graphs obtained by considering all subgraphs of G and taking the component containing v .

2.2. Self-Avoiding Walk Tree Representation

Since our work builds on that of Weitz’s, we first describe the self-avoiding walk (SAW) tree representation introduced in [33]. Given $G = (V, E)$, we first fix an arbitrary ordering $>_w$ on the neighbors of each vertex w in G . For each $v \in V$, the tree $T_{\text{saw}}(G, v)$ is constructed as follows. Consider the tree T of self-avoiding walks originating from v , additionally including the vertices closing a cycle as leaves of the tree. We then fix such leaves of T to be occupied or unoccupied in the following manner. If a leaf vertex closes a cycle in G , say $w \rightarrow v_1 \rightarrow \dots \rightarrow v_\ell \rightarrow w$, then if $v_1 >_w v_\ell$ we fix this leaf to be unoccupied, otherwise if $v_1 <_w v_\ell$ we fix the leaf to be occupied. Note, if the leaf is fixed to be unoccupied we simply remove that vertex from the tree. If the leaf is fixed to be occupied, we remove that leaf and all of its neighbors, i.e. we remove the parent of that leaf from the tree. The resulting tree is denoted as $T_{\text{saw}} = T_{\text{saw}}(G, v)$. See Figure 1 for an illustration of T_{saw} for a particular example.

Weitz [33] proves the following theorem for the hard-core model, which shows that the marginal distribution at the root in $T_{\text{saw}}(G, v)$ is identical to the marginal distribution for v in G . For a graph $G = (V, E)$, a subset $S \subset V$ and configuration ρ on S , for $T_{\text{saw}} = T_{\text{saw}}(G, v)$, let ρ in T_{saw} denote the configuration on S in T_{saw} where for $w \in S$ every occurrence of w in T_{saw} is assigned according to ρ .

Theorem 1 (SAW Tree Representation, Theorem 3.1 in [33]): For any graph $G = (V, E)$, $v \in V$, $\lambda > 0$, and configuration ρ on $S \subset V$, for $T = T_{\text{saw}}(G, v)$ the following holds:

$$\alpha_{G,v}^\rho = \alpha_{T,v}^\rho.$$

Note, the tree $T_{\text{saw}}(G, v)$ preserves the distance of vertices from v in G , which implies the following corollary.

Corollary 2: If SSM holds with rate γ for $T_{\text{saw}}(G, v)$ for all v , then SSM holds for G with rate γ .

The reverse implication of Corollary 2 does not hold since there are configurations on S in T_{saw} which are not necessarily realizable in G . Observe that if G has maximum degree Δ , any SAW tree of G is a subtree of the regular tree of degree Δ .

2.3. Our Proof Approach

In summary, Weitz [33] first shows (via Theorem 1) that to prove SSM holds on a graph $G = (V, E)$, it suffices to prove SSM holds on the trees $T_{\text{saw}}(G, v)$, for all $v \in V$. Weitz then proves that the regular tree \mathbb{T}_Δ ‘‘dominates’’ every tree of maximum degree Δ in the sense that, for all trees of maximum degree Δ , SSM holds when $\lambda < \lambda_c(\mathbb{T}_\Delta)$. We refine this second part of Weitz’s approach. In particular,

For example, the family $\mathcal{F}_{\leq M}$ with $M = [\Delta]$ includes the family of trees with maximum branching Δ . On the other hand, $\mathcal{F}_{\leq M}$ with $M = \begin{pmatrix} 0 & \Delta + 1 \\ 0 & \Delta \end{pmatrix}$ describes the family of graphs of maximum degree $\Delta + 1$, by assigning the root of tree $T \in \mathcal{F}_{\leq M}$ to be of type 1 and the other vertices of the tree to be of type 2. Note that if M has maximum degree Δ , then every $G \in \mathcal{F}_{\leq M}$ also has maximum degree Δ .

In this framework, Weitz's result establishing SSM for all graphs of maximum degree Δ when $\lambda < \lambda_c(\mathbb{T}_\Delta)$ can be stated as establishing SSM with uniform rate for all $G \in \mathcal{F}_{\leq M}$ with $M = \begin{pmatrix} 0 & \Delta \\ 0 & \Delta - 1 \end{pmatrix}$; and we are interested in establishing its analogy for general M . To this end, we will use the following notion of SSM for M .

Remark 1: To establish SSM for M , it suffices to prove that SSM holds with uniform rate for all trees in $\mathcal{F}_{\leq M}$ due to Corollary 2. In addition, note that SSM holds for $M = \begin{pmatrix} 0 & \Delta + 1 \\ 0 & \Delta \end{pmatrix}$ if and only if it holds for (Δ) since the root of a tree $T \in \mathcal{F}_{\leq M}$ is the only possible vertex of type 1 in T .

Finally, we define SSM for a branching matrix M .

Definition 4: Given a branching matrix M , we say SSM holds for M if SSM holds with uniform rate for all $G \in \mathcal{F}_{\leq M}$.

Remark 2: To establish SSM for M , it suffices to prove that SSM holds with uniform rate for all trees in $\mathcal{F}_{\leq M}$ due to Corollary 2.

3.2. Implications of SSM

We present a new approach for proving SSM for a branching matrix M . There are multiple consequences of SSM for M as summarized in the following theorem. We first state some definitions needed for stating the theorem.

Following Goldberg et al. [15] we use the following variant of amenability for infinite graphs. Here we consider an infinite graph $G = (V, E)$. For $v \in V$ and a non-negative integer d , let $B_d(v)$ denote the set of vertices within distance $\leq d$ from v , where distance is the length of the shortest path. For a set of vertices S , the (outer) boundary and neighborhood amenability are defined, respectively, as:

$$\partial S := \{w \in V : w \notin S, \text{ and } w \text{ has a neighbor } y \in S\}$$

and $r_d = \sup_{v \in V} \frac{|\partial B_d(v)|}{|B_d(v)|}$. The infinite graph is said to be *neighborhood-amenable* if $\inf_d r_d = 0$.

Now we can state the following theorem detailing the implications of SSM of interest to us.

Theorem 3: For a $t \times t$ branching matrix M , if SSM holds for M then the following hold:

- 1) For every $G \in \mathcal{F}_{\leq M}$, SSM holds on G .
- 2) For every infinite graph $G \in \mathcal{F}_{\leq M}$, there is a unique infinite-volume Gibbs measure on G .

- 3) If M has maximum degree Δ , if $t = O(1)$ and $\Delta = O(1)$, then for every (finite) $G \in \mathcal{F}_{\leq M}$, Weitz's algorithm [33] gives an FPAS for approximating the partition function $Z(G)$.
- 4) For every infinite $H \in \mathcal{F}_{\leq M}$ which is neighborhood-amenable, for every finite subgraph $G = (V, E)$ of H , the Glauber dynamics has $O(n^2)$ mixing time. Moreover, if $H = \mathbb{Z}^d$ for constant d , then for every finite subgraph $G = (V, E)$ of H , the Glauber dynamics has $O(n \log n)$ mixing time.

See [36] for the proof of Theorem 3.

4. ESTABLISHING SSM FOR BRANCHING MATRICES

In this section we present a sufficient condition implying SSM for the family of trees generated by a branching matrix. As a consequence of the approach presented in this section we get a simpler proof of Weitz's result [33] implying SSM for all graphs with maximum degree Δ when $\lambda < \lambda_c(\mathbb{T}_\Delta)$. We then apply the condition presented in this section to \mathbb{Z}^2 in Section 5.

To show the decay of influence of a boundary condition ρ , a common strategy is to prove some form of contraction for the 'one-step' iteration given in (1) below. More generally, we will prove such a contraction for an appropriate set of 'statistics' of the unoccupied marginal probability.

A *statistic* of the univariate parameter $x \in [a, b]$ is a monotone (i.e., strictly increasing or decreasing) function $\varphi : [a, b] \rightarrow \mathbb{R}$. For a $t \times t$ branching matrix M we consider a set of t statistics $\varphi_1, \dots, \varphi_t$, one for each type. For the simpler case when $M = [\Delta]$ and hence $t = 1$, we have a single statistic φ . Our aim is proving contraction for an appropriate set of statistics of the probability that the root of a tree is unoccupied.

We first focus on the case of a single type. Consider a tree $T = (V, E) \in \mathcal{F}_{\leq M}$ with root r . For $v \in V$, let $N(v)$ denote the children of v , and let $d(v) := |N(v)|$ the number of children. Let T_v denote the subtree rooted at v . We will analyze the unoccupied probability for a vertex v , but v will always be the root of its subtree. Hence, to simplify the notation, for a boundary condition ρ on $S \subset V$, let $\alpha_v^\rho = \alpha_{T_v, v}^\rho$.

A straightforward recursive calculation with the partition function leads to the following relation:

$$\alpha_v^\rho = \begin{cases} \frac{1}{1+\lambda} & \text{if } N(v) = \emptyset \\ \frac{1}{1+\lambda \prod_{w \in N(v)} \alpha_w^\rho} & \text{otherwise.} \end{cases} \quad (1)$$

Note, the unoccupied probability always lies in the interval $I := \left[\frac{1}{1+\lambda}, 1 \right]$, i.e., for all v , all ρ , $\alpha_v^\rho \in I$.

For $v \in V$, let $m_v^\rho := \varphi(\alpha_v^\rho)$ be the 'message' at vertex

v. The messages satisfy the following recurrence:

$$\begin{aligned} m_v^\rho &= \varphi \left(\frac{1}{1 + \lambda \prod_{w \in N(v)} \alpha_w^\rho} \right) \\ &= \varphi \left(\frac{1}{1 + \lambda \prod_{w \in N(v)} \varphi^{-1}(m_w^\rho)} \right). \end{aligned}$$

Our aim is to prove uniform contraction of the messages on all trees $T \in \mathcal{F}_{\leq M}$. To this end, we will consider a more general set of messages. Namely, we consider messages m_1, \dots, m_Δ where for every $1 \leq i \leq \Delta$, $m_i = \varphi(\alpha_i)$ and $\alpha_i \in I := \left[\frac{1}{1+\lambda}, 1 \right]$. This set of tuples $\alpha_1, \dots, \alpha_\Delta \in I$ contains all of the tuples obtainable on a tree.

For $\alpha_1, \dots, \alpha_\Delta \in I$, let $m_i = \varphi(\alpha_i)$, $1 \leq i \leq \Delta$, and let

$$F(m_1, \dots, m_\Delta) := \varphi \left(\frac{1}{1 + \lambda \prod_{i=1}^{\Delta} \varphi^{-1}(m_i)} \right).$$

Ideally, we would like to establish the following contraction: there exists a $0 < \gamma < 1$ such that for all $\alpha_1, \dots, \alpha_\Delta, \alpha'_1, \dots, \alpha'_\Delta \in I$,

$$|F(m_1, \dots, m_\Delta) - F(m'_1, \dots, m'_\Delta)| \leq \gamma \max_{1 \leq i \leq \Delta} |m_i - m'_i|,$$

where $m_i = \varphi(\alpha_i)$ and $m'_i = \varphi(\alpha'_i)$. We will instead show that the following weaker condition suffices. Namely, that the desired contraction holds for all $|\alpha_i - \alpha'_i| \leq \epsilon$ for some $\epsilon > 0$. This is equivalent to the following condition.

Definition 5: Let $I = \left[\frac{1}{1+\lambda}, 1 \right]$. For the branching matrix $M = [\Delta]$, we say that *Condition* (\star) is satisfied if for all $\alpha_1, \dots, \alpha_\Delta \in I$, by setting $m_i = \varphi(\alpha_i)$ for $1 \leq i \leq \Delta$, the following holds:

$$\|\nabla F(m_1, \dots, m_\Delta)\|_1 = \sum_{i=1}^{\Delta} \left| \frac{\partial F(m_1, \dots, m_\Delta)}{\partial m_i} \right| < 1. \quad (\star)$$

Let us now consider a natural generalization of the above notion for a branching matrix with multiple types. Let M be a $t \times t$ branching matrix. For $1 \leq \ell \leq t$, let $\Delta_\ell = \sum_{k=1}^t M_{\ell k}$ denote the maximum number of children of a vertex of type ℓ . Once again, consider a tree $T = (V, E) \in \mathcal{F}_{\leq M}$ with root r . For $v \in V$, let $t(v)$ denote its type. As before, $N(v)$ are the children of v , $d(v)$ is the number of children of v , and for a boundary condition ρ on $S \subset V$, α_v^ρ is the unoccupied probability for v in the tree T_v under ρ .

The recursive calculation in (1) for α_v in terms of α_w , $w \in N(v)$, still holds. For the case of multiple types, for $v \in V$, let $m_v^\rho := \varphi_{t(v)}(\alpha_v^\rho)$ be the message at vertex v . The messages satisfy the following recurrence:

$$m_v^\rho = \varphi_{t(v)} \left(\frac{1}{1 + \lambda \prod_{w \in N(v)} \varphi_{t(w)}^{-1}(m_w^\rho)} \right).$$

For each type $1 \leq \ell \leq t$, we consider contraction of messages derived from all $\alpha_1, \dots, \alpha_{\Delta_\ell} \in I$. We need to identify

the type of each these quantities α_i in order to determine the appropriate statistic to apply. The assignment of types needs to be consistent with the branching matrix M . Hence, let $s_\ell : \{1, \dots, \Delta_\ell\} \rightarrow \{1, \dots, t\}$ be the following assignment. Let $M_{\ell, \leq 0} = 0$ and for $1 \leq i \leq t$, let $M_{\ell, \leq i} = \sum_{k=1}^i M_{\ell, k}$. For $1 \leq i \leq t$, for $M_{\ell, \leq i-1} < j \leq M_{\ell, \leq i}$, let $s_\ell(j) = i$.

For type $1 \leq \ell \leq t$, for $\alpha_1, \dots, \alpha_{\Delta_\ell} \in I$, set $m_j = \varphi_{s_\ell(j)}(\alpha_j)$, $1 \leq j \leq \Delta_\ell$, and let

$$F_\ell(m_1, \dots, m_{\Delta_\ell}) := \varphi_\ell \left(\frac{1}{1 + \lambda \prod_{j=1}^{\Delta_\ell} \varphi_{s_\ell(j)}^{-1}(m_j)} \right).$$

Note,

$$m_v^\rho = F_{t(v)} \left(m_{w_1}^\rho, \dots, m_{w_{d(v)}}^\rho \right), \quad (2)$$

where $N(v) = \{w_1, \dots, w_{d(v)}\}$.¹

We generalize *Condition* (\star) to branching matrices with multiple types by allowing a weighting of the types by parameters c_1, \dots, c_t .

Definition 6: Let $I = \left[\frac{1}{1+\lambda}, 1 \right]$. For a $t \times t$ branching matrix M , we say that *Condition* $(\star\star)$ is satisfied if there exist c_1, \dots, c_t , such that for all $1 \leq \ell \leq t$, for all $\alpha_1, \dots, \alpha_{\Delta_\ell} \in I$, by setting $m_i = \varphi_{s_\ell(i)}(\alpha_i)$ for $1 \leq i \leq \Delta_\ell$, the following holds:

$$\sum_{i=1}^{\Delta_\ell} c_{s_\ell(i)} \left| \frac{\partial F_\ell(m_1, \dots, m_{\Delta_\ell})}{\partial m_i} \right| < c_\ell. \quad (\star\star)$$

The following lemma establishes a sufficient condition so that SSM holds for M .

Lemma 4: For a $t \times t$ branching matrix M , if for every $1 \leq \ell \leq t$, φ_ℓ is continuously differentiable on the interval $I = \left[\frac{1}{1+\lambda}, 1 \right]$ and $\inf_{x \in I} |\varphi'_\ell(x)| > 0$, and if *Condition* (\star) is satisfied for $t = 1$ or *Condition* $(\star\star)$ is satisfied for $t \geq 2$ then SSM holds for M , and hence the conclusions of *Theorem 3* follow.

See [36] for the proof of *Lemma 4*.

4.1. Reproving Weitz's Result of SSM for Trees

In this section, we aim at finding a good choice of statistics. First we find such a statistic for the case $M = [\Delta]$, i.e., the case of a single type, which enables us to reprove Weitz's result [33] that when $\lambda < \lambda_c(\mathbb{T}_\Delta)$ SSM holds for every tree of maximum degree Δ .

Using *Lemma 4* (and the simpler condition (\star) for the case of a single type) we obtain a simpler proof of Weitz's result [33] that for every tree T with maximum degree $\Delta + 1$ (hence, for every graph G of maximum degree $\Delta + 1$) and for all $\lambda < \lambda_c(\mathbb{T}_{\Delta+1}) = \Delta^\Delta / (\Delta - 1)^{\Delta+1}$, SSM holds on T (and on G).

¹Strictly speaking, F_ℓ requires Δ_ℓ arguments, so for (2) to hold in the case when $d(v) < \Delta_\ell$ we can simply add additional arguments corresponding to $\alpha = 1$, which fixes these additional vertices to be unoccupied (and therefore absent).

Theorem 5: Let $\varphi(x) = \frac{1}{s} \log\left(\frac{x}{s-x}\right)$ where $s = \frac{\Delta+1}{\Delta}$. Then, Condition (\star) holds for $M = [\Delta]$ and $\lambda < \lambda_c(\mathbb{T}_{\Delta+1})$. Consequently, SSM and the conclusions of Theorem 3 hold for $M = \begin{pmatrix} 0 & \Delta+1 \\ 0 & \Delta \end{pmatrix}$ and $\lambda < \lambda_c(\mathbb{T}_{\Delta+1})$.

See [36] for the proof of Theorem 5.

4.2. DMS Condition: A Sufficient Criterion

Theorem 5 suggests choosing $\varphi_j(x) = \frac{1}{s_j} \log\left(\frac{x}{s_j-x}\right)$ with appropriate parameters s_j for a general branching matrix M . Under this choice, we obtain the following condition for SSM.

Definition 7 (DMS Condition): Given a $t \times t$ branching matrix M and $\lambda^* > 0$, for $s_1, \dots, s_t > 1$ and $\mathbf{c} = (c_1, \dots, c_t) > 0$, let D and S be the diagonal matrices defined as

$$D_{jj} = \sup_{\alpha \in [\frac{1}{1+\lambda^*}, 1]} \frac{(1-\alpha) \left(1 - \theta_j \left(\frac{1-\alpha}{\lambda^* \alpha}\right)^{1/\Delta_j}\right)}{s_j - \alpha}$$

$$S_{jj} = s_j,$$

where

$$\theta_j := \frac{\left(\prod_{\ell} c_{\ell}^{M_{j\ell}}\right)^{1/\Delta_j}}{\sum_{\ell} c_{\ell} s_{\ell} M_{j\ell} / \Delta_j} \quad \text{and} \quad \Delta_j = \sum_{\ell} M_{j\ell}.$$

We say the *DMS Condition holds for M and λ^** if there exist $s_1, \dots, s_t > 1$ and $\mathbf{c} > 0$ such that:

$$(DMS) \mathbf{c} < \mathbf{c}.$$

Theorem 6: If the DMS Condition holds for M and $\lambda^* > 0$, then Condition $(\star\star)$ holds with the choice of $\varphi_j(x) = \frac{1}{s_j} \log\left(\frac{x}{s_j-x}\right)$ for all $\lambda \leq \lambda^*$. Consequently, SSM and the conclusions of Theorem 3 hold for M and all $\lambda \leq \lambda^*$.

Proof: First, one can check that

$$\left| \frac{\partial F_j}{\partial m_i} \right| = \frac{1-\alpha}{s_j - \alpha} (s_{j_i} - \alpha_i),$$

where $\alpha_i = \varphi_{j_i}^{-1}(m_i)$ and $\alpha = \frac{1}{1+\lambda \prod_{i=1}^{\Delta_j} \alpha_i}$.

Hence, it follows that

$$\begin{aligned} \sum_{i=1}^{\Delta_j} c_{j_i} \left| \frac{\partial F_j}{\partial m_j} \right| &= \frac{1-\alpha}{s_j - \alpha} \sum_{i=1}^{\Delta_j} c_{j_i} (s_{j_i} - \alpha_i) \\ &\leq \frac{1-\alpha}{s_j - \alpha} \left(\sum_{i=1}^{\Delta_j} c_{j_i} s_{j_i} - \Delta_j \left(\prod_{i=1}^{\Delta_j} c_{j_i} \alpha_i \right)^{1/\Delta_j} \right) \\ &\quad \text{by the arithmetic-geometric mean ineq.} \\ &= \frac{1-\alpha}{s_j - \alpha} \left(\sum_{i=1}^{\Delta_j} c_{j_i} s_{j_i} - \Delta_j \left(\prod_{i=1}^{\Delta_j} c_{j_i} \right)^{1/\Delta_j} \left(\frac{1-\alpha}{\lambda \alpha} \right)^{1/\Delta_j} \right) \\ &= \frac{1-\alpha}{s_j - \alpha} \left(1 - \theta_j \left(\frac{1-\alpha}{\lambda \alpha} \right)^{1/\Delta_j} \right) \sum_{i=1}^{\Delta_j} c_{j_i} s_{j_i} \\ &\quad \text{by the definition of } \theta_j \\ &\leq \frac{1-\alpha}{s_j - \alpha} \left(1 - \theta_j \left(\frac{1-\alpha}{\lambda^* \alpha} \right)^{1/\Delta_j} \right) \sum_{i=1}^{\Delta_j} c_{j_i} s_{j_i} \\ &\leq D_{jj} \sum_{\ell} M_{j\ell} c_{\ell} s_{\ell} \quad \text{by the definition of } D_{jj} \\ &< c_j \quad \text{by the DMS condition.} \end{aligned}$$

which satisfies the desired condition $(\star\star)$ of Lemma 4. This completes the proof of Theorem 6. \blacksquare

5. APPLICATION TO \mathbb{Z}^2 IN THE HARD-CORE MODEL

In this section, we show how to apply Theorem 6 and Theorem 3 to the two-dimensional integer lattice \mathbb{Z}^2 and improve the lower bound on $\lambda_c(\mathbb{Z}^2)$, resulting in the following theorem.

Theorem 7: There exists a $t \times t$ matrix M such that $T_{\text{saw}}(\mathbb{Z}^2) \in \mathcal{F}_{\leq M}$ and the DMS Condition holds for $\lambda^* = 2.3882$.

Therefore, the following hold for \mathbb{Z}^2 for all $\lambda \leq \lambda^*$:

- 1) SSM holds on \mathbb{Z}^2 .
- 2) There is a unique infinite-volume Gibbs measure on \mathbb{Z}^2 .
- 3) If M has maximum degree Δ , if $t = O(1)$ and $\Delta = O(1)$, then for every finite subgraph G of \mathbb{Z}^2 , Weitz's algorithm [33] gives an FPAS for approximating the partition function $Z(G)$.
- 4) For every finite subgraph G of \mathbb{Z}^2 , the Glauber dynamics has $O(n \log n)$ mixing time.

We first illustrate our approach by showing that Theorem 7 holds with $\lambda^* = 1.8801$ for a simple choice of M . We then explain how to extend the approach to higher λ .

The graph \mathbb{Z}^2 is translation-invariant, hence the tree $T_{\text{saw}}(\mathbb{Z}^2, v)$ is identical for every vertex $v \in \mathbb{Z}^2$. Fix a vertex, call it the origin \mathbf{o} , and let us consider $T_{\text{saw}}(\mathbb{Z}^2) = T_{\text{saw}}(\mathbb{Z}^2, \mathbf{o})$. Each path from the root of $T_{\text{saw}}(\mathbb{Z}^2)$ corresponds to a self-avoiding walk in \mathbb{Z}^2 starting at the origin. Any walk on \mathbb{Z}^2 starting at the origin \mathbf{o} can be encoded as

a string over the alphabet $\{N, E, S, W\}$ corresponding to North, East, South and West. The tree $T_{\text{saw}}(\mathbb{Z}^2)$ contains such strings, truncated the first time the corresponding walk completes a cycle. A relaxed notion of such a tree would be to truncate a walk only when a 4-cycle is completed. Denote such a tree by T_4 , and clearly we have that $T_{\text{saw}}(\mathbb{Z}^2)$ is a subtree of T_4 . Our first idea is to define a branching matrix N so that $T_4 \in \mathcal{F}_{\leq N}$, and hence $T_{\text{saw}}(\mathbb{Z}^2) \in \mathcal{F}_{\leq N}$.

To avoid cycles of length four, it is enough to track the last three steps of the walks. Labeling the paths using $\{N, E, S, W\}$ as mentioned above, their branching rule is easily determined. For example, a path labeled NWS is followed by paths labeled WSW and WSS corresponding to adding the directions W and S to the path, while adding the direction E would have resulted in a cycle of length 4. The number of types in the corresponding branching matrix is $\leq 4 + 4^2 + 4^3 \leq 5^3$. Indeed, we can reduce the representation of such paths by using isomorphisms between the generating rules among them. This results in 4 types in the following branching matrix N :

$$N = \begin{pmatrix} 0 & 4 & 0 & 0 \\ 0 & 1 & 2 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}, \quad (3)$$

where the type $i = 0, \dots, 3$ of a vertex (walk) in the tree represents the fact that a continuation with a minimum of $4 - i$ additional edges are needed to complete a cycle of length 4.

See Figure 2 for an illustration of this branching matrix N . One can verify that this branching matrix captures, inter alia, the self-avoiding walk trees from \mathbb{Z}^2 :

Observation 2: For any finite subgraph $G = (V, E)$ of \mathbb{Z}^2 and $v \in V$, $T_{\text{saw}}(G, v) \in \mathcal{F}_{\leq N}$.

For this branching matrix, one can check that the (DMS) condition of Theorem 6 holds with $\lambda^* = 1.8801$, $\mathbf{S} = \text{Diag}(1.040, 1.388, 1.353, 1.255)$ and $\mathbf{c} = (0.266037, 0.100891, 0.100115, 0.0973861)$. Checking the DMS Condition for a given choice of parameters would have been a straightforward task, were it not for the irrationality of the coefficients D_{jj} . However, one can establish rigorous upper bounds for D_{jj} , based on concavity of the function (of α) used in the definition of D_{jj} , in a suitable range of the parameters. These details will be discussed further below. As a consequence, we can conclude that Theorem 7 holds for N and $\lambda^* = 1.8801$.

The primary reason why the branching matrix N improves beyond the tree-threshold of $\lambda < \lambda_c(\mathbb{T}_4) = 27/16 = 1.6875$ is that the average branching factor of any $T \in \mathcal{F}_{\leq N}$ is significantly smaller than that of the regular tree of degree 4.

To obtain a further reduction in the average branching, we observe that N did not consider the effect of occupying (or unoccupying) certain leaves as prescribed in Weitz's

construction. Starting with T_4 , prune the leaves as is done in the construction of $T_{\text{saw}}(\mathbb{Z}^2)$ from Section 2.2. Denote the new tree as T'_4 . Clearly we still have that $T_{\text{saw}}(\mathbb{Z}^2)$ is a subtree of T'_4 .

Let us illustrate the difference between T_4 and the pruned tree T'_4 . We first fix an underlying order for the neighbors of each vertex. To this end, say $N > E > S > W$ and this prescribes an ordering of the neighbors of each vertex. Consider a leaf vertex v' in the tree T_4 corresponding to the vertex v in \mathbb{Z}^2 and to the path ρ in \mathbb{Z}^2 . Since v' is a leaf vertex in T_4 , ρ must end with a cycle at v , say $WNES$. Since v was exited in the West direction at the beginning of the 4-cycle, and since $W < N$, the leaf vertex v' would be labeled occupied in Weitz's construction, thus resulting in the removal of v' and its parent in the construction of T'_4 . Note, every vertex w' in T_4 of type WNE has a child v' of type NES , and consequently w' (and its subtree) will be removed from the tree in the pruning process to construct T'_4 . Thus, after removing vertices of type WNE (and similarly, WSE , SEN and ENW) from T_4 , it is still the case that $T_{\text{saw}}(\mathbb{Z}^2)$ is a subtree of the resulting tree (T'_4). This highlights why T'_4 has a significantly smaller average branching factor than T_4 .

We can define a branching matrix M_2 , with 17 types (as illustrated in Figure 3), such that $T'_4 \in \mathcal{F}_{\leq M_2}$, and hence $T_{\text{saw}}(\mathbb{Z}^2) \in \mathcal{F}_{\leq M_2}$. We can prove the DMS Condition is satisfied for M_2 at $\lambda^* = 2.1625$, as we will describe shortly, which significantly improves upon our initial bound resulting from considering T_4 .

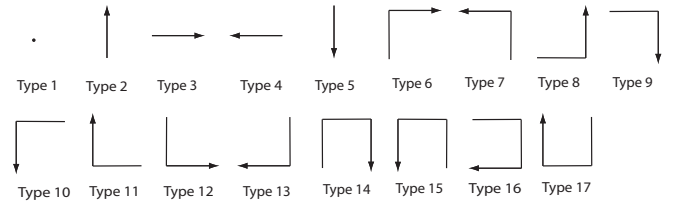


Figure 3. Shapes that the seventeen types (or labels) represent for M_2 where $T'_4 \in \mathcal{F}_{\leq M_2}$.

A natural direction for improved results is to consider branching matrices corresponding to avoidance of larger cycles, while also accounting for the removal of vertices prescribed by the construction of Weitz. We briefly outline such an approach for walks avoiding cycles of length at most 4, 6, and 8, respectively. Avoiding cycles of length $2i$ results in $\sum_{j \leq 2i-1} 4^j \leq 5^{2i-1}$ types, hence the computations become increasingly difficult for larger i . For 8-cycles the task of finding appropriate parameters to satisfy the conditions of Theorem 6 is still feasible.

More precisely, we can define branching matrices M_i for $i \geq 2$, that (i) represent the structure of trees of walks avoiding cycles of length $\leq 2i$, as well as (ii) account for

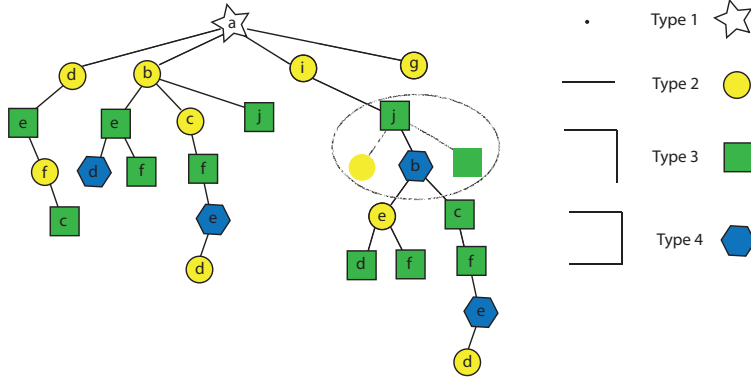


Figure 2. Assignment of the four types from matrix N defined in (3) to the self-avoiding walk tree T_{saw} from Figure 1. In the circled area, we also draw redundant leaves at vertex j which may appear in the branching rule, but not in T_{saw} .

the removal of vertices based on children being labeled ‘occupied.’ One can extend the above construction of M_2 for general $i > 2$ by using types encoded by longer paths with length at most $2i$ and ruling out the types that either contain a cycle of length at most $2i$ or whose children end up being labeled occupied. We can make the following general observation from our construction.

Observation 3: For any finite subgraph $G = (V, E)$ of \mathbb{Z}^2 and $v \in V$, $T_{\text{saw}}(G, v) \in \mathcal{F}_{\leq M_i}$ for any $i \geq 2$.

As mentioned earlier, the matrix M_2 constructed above consists of 17 types. An explicit description of it is shown in the Online Appendix [34], along with the associated parameters \mathcal{S} and \mathbf{c} for which one can check the DMS Condition for $\lambda^* = 2.1625$; this establishes Theorem 7 for M_2 and $\lambda^* = 2.1625$.

The following table summarizes the threshold λ^* we obtain for each M_i :

(a, b, c)	λ^*
(4, No, 4)	1.8801
(4, Yes, 17)	2.1625
(6, Yes, 132)	2.3335
(8, Yes, 922)	2.3882

In above, a, b and c indicate the max length of avoiding-cycles, effect of occupations and number of types, respectively.

Note that, one can further improve the bound on λ by using more types for higher i and hence Theorem 7 on \mathbb{Z}^2 will hold with the corresponding activity λ^* . For any such matrix, the verification of the DMS Condition relies on (i) ‘guessing’ appropriate values for the parameters \mathcal{S} and \mathbf{c} and (ii) formally verifying that DMS Condition holds for the chosen \mathcal{S} and \mathbf{c} . In choosing desirable \mathcal{S} and \mathbf{c} , we employed a heuristic random walk algorithm.

To verify that the DMS Condition holds for a given *rational* matrix \mathcal{S} and vector \mathbf{c} is straightforward, provided we can obtain a rational upper bound for each type j for the

function:

$$f_j(\alpha) = \frac{(1 - \alpha) \left(1 - \theta_j \left(\frac{1 - \alpha}{\lambda \alpha}\right)^{1/\Delta_j}\right)}{s_j - \alpha}.$$

Indeed, due to the concavity of this function for $0 < \theta_j \leq 1$, $s_j > 51/50$ and $\lambda > 27/16$,² it is always possible to find a *provable* upper bound for f_j in such a regime. This can be done, for example, by describing a suitable ‘envelope’ for f_j consisting of a piecewise linear function of the form:

$$g_j(\alpha) = \begin{cases} B_\ell & \text{if } \alpha < \alpha_\ell \\ \min \left\{ b_\ell (\alpha - \alpha_\ell) + B_\ell, \right. & \text{if } \alpha_\ell < \alpha < \alpha_u \\ \left. b_u (\alpha - \alpha_u) + B_u \right\} & \\ B_u & \text{if } \alpha > \alpha_u \end{cases}$$

where α_ℓ, α_u are points such that $b_\ell > f'_j(\alpha_\ell) > 0$, $b_u < f'_j(\alpha_u) < 0$, $B_\ell > f_j(\alpha_\ell)$ and $B_u > f_j(\alpha_u)$. It is clear for any such function that $g_j(\alpha) > f_j(\alpha)$, thus we obtain a provable upper bound for f_j using g_j .

For every M_i in the above table, we provide \mathcal{S} and \mathbf{c} , along with appropriate envelopes that lead to upper bounds \widehat{D}_{jj} for the corresponding D_{jj} . Then we verify that the DMS Condition holds for the given values of λ by replacing D_{jj} with \widehat{D}_{jj} . For $i = 2, 3, 4$ these values (M , \mathcal{S} , \mathbf{c} , α_ℓ and α_u) are given in the Online Appendix [34].

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²This is a nontrivial algebraic fact. It can be proved by transforming the second derivatives condition to a set of integer polynomial constraints and using the ‘**resolve**’ function in MATHEMATICA for the satisfiability of the constraints, which is rigorous by the Tarski-Seidenberg Theorem [31] for the real polynomial systems [35] and the so-called cylindrical algebraic decomposition [2].

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- [34] Data is available from:
<http://www.cc.gatech.edu/~vigoda/hardcore.html>
- [35] See: <http://reference.wolfram.com/mathematica/tutorial/RealPolynomialSystems.html>
- [36] The full version is available from the arXiv at: <http://arxiv.org/abs/1105.0914>