Inference and Sampling of K_{33}-free Ising Models

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Abstract

We call an Ising model tractable when it is possible to compute its partition function value (statistical inference) in polynomial time. The tractability also implies an ability to sample configurations of this model in polynomial time. The notion of tractability extends the basic case of planar zero-field Ising models. Our starting point is to describe algorithms for the basic case, computing partition function and sampling efficiently. Then, we extend our tractable inference and sampling algorithms to models whose triconnected components are either planar or graphs of $O(1)$ size. In particular, it results in a polynomial-time inference and sampling algorithms for K_{33} (minor)-free topologies of zero-field Ising models—a generalization of planar graphs with a potentially unbounded genus.

1. Introduction

Computing the partition function of the Ising model is generally intractable, even an approximate solution in the special anti-ferromagnetic case of arbitrary topology would have colossal consequences in the complexity theory (Jerrum & Sinclair, 1993). Therefore, a question of interest—rather than addressing the general case—is to look after tractable families of Ising models. In the following, we briefly review tractability related to planar graphs and graphs embedded in surfaces of small genus.

Related work. Onsager (1944) gave a closed-form solution for the partition function in the case of a homogeneous interaction Ising model over an infinite two-dimensional square grid without a magnetic field. This result has opened an exciting era of phase transition discoveries, which is arguably one of the most significant contributions in theoretical and mathematical physics of the 20th century. Then, Kac and Ward (1952) showed in the case of a finite square lattice that the problem of the partition function computation is reducible to a determinant. Kasteleyn (1963) generalized the results to the case of an arbitrary inhomogeneous interaction Ising model over an arbitrary planar graph. Kasteleyn's construction was based on mapping of the Ising model to a perfect matching (PM) model with specially defined weights over a modified graph. Kasteleyn's construction was also based on the so-called Pfaffian orientation, which allows counting of PMs by finding a single Pfaffian (or determinant) of a matrix. Fisher (1966) simplified Kasteleyn's construction such that the modified graph remained planar. Transition to PM is fruitful because it extends planar zero-field Ising model inference to models embedded on a torus (Kasteleyn, 1963) and, in fact, on any surface of small (orientable) genus g, but with a price of the additional, multiplicative, and exponential in genus, 4^g, factor in the algorithm's run time (Gallucio & Loebl, 1999).

A parallel way of reducing the planar zero-field Ising model to a PM problem consists of constructing a so-called expanded dual graph (Bieche et al., 1980; Barahona, 1982; Schraudolph & Kamenetsky, 2009). This approach is more natural and interpretable because there is a one-to-one correspondence between spin configurations and PMs on the expanded dual graph. An extra advantage of this approach is that the reduction allows one to develop an exact efficient sampling. Based on linear algebra and planar separator theory (Lipton & Tarjan, 1979), Wilson introduced an algorithm (1997) that allows one to sample PMs over planar graphs in $O(N^{\frac{3}{2}})$ time. The algorithms were implemented in (Thomas & Middleton, 2009; 2013) for the Ising model sampling, however, the implementation was limited to only the special case of a square lattice. In (Thomas & Middleton, 2009) a simple extension of the Wilson's algorithm to the case of bounded genus graphs was also suggested, again with the 4^g factor in complexity. Notice that imposing zero field condition is critical, as otherwise, the Ising model over a planar graph is NP-hard (Barahona, 1982). On the other hand, even in the case of zero magnetic field Ising models over general graphs are difficult (Barahona, 1982).

Contribution. In this manuscript, we discuss tractability related to the Ising model with zero magnetic fields over

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Proceedings of the 36^{th} International Conference on Machine Learning, Long Beach, California, PMLR 97, 2019.

graphs more general than planar. Our construction is related to graphs characterized in terms of their excluded minor property. Planar graphs are characterized by excluded K_5 minor and K_{33} minor (Wagner's theorem (Diestel, 2006), Chapter 4.4). Therefore, instead of attempting to generalize from planar to graphs embedded into surfaces of higher genus, it is natural to consider generalizations associated with a family of graphs excluding K_5 minor or K_{33} minor.

In this manuscript, we show that K_{33}-free zero-field Ising models are tractable in terms of inference and sampling and give a tight asymptotic bound, $O(N^{\frac{3}{2}})$, for both operations. For that purpose, we use graph decomposition into triconnected components—the result of recursive splitting by pairs of vertices, disconnecting the graph. Indeed, the K_{33}-free graphs are simple to work with because their triconnected components are either planar or K_5 graphs (Hall, 1943). Therefore, the essence of our construction is to decompose the inference task in Ising over a K_{33}-free graph into a sequential dynamic programming evaluation over planar or K_5 graphs in the spirit of (Straub et al., 2014). Notice that the triconnected classification of the tractable zero-field Ising models is complementary to the aforementioned small genus classification. We illustrate the difference between the two classifications with an explicit example of a tractable problem over a graph with genus growing linearly with graph size.

Structure. The manuscript is organized as follows. Sections 2 and 3, respectively, establish notations and pose problems of inference and sampling. Section 4 presents transition from the zero-field Ising model to an equivalent tractable perfect matching (PM) model. This provides a description of a $O(N^{\frac{3}{2}})$ inference and sampling method in planar models, which is new (to the best of our knowledge), and it sets the stage for what follows. Section 5 discusses a scheme for polynomial inference and sampling in zero-field models over graphs with triconnected components that are either planar or of $O(1)$ size. Section 6 applies this scheme to K_{33}-free zero-field Ising models, resulting in tight asymptotic bounds, which appear to be equivalent to those in the planar case. Section 7 describes benchmarks justifying correctness and efficiency of our algorithm. Technical proofs of statements given throughout the manuscript can be found in the supplementary material.

2. Definitions and Notations

Let $V = \{v_1, ..., v_{|V|}\}$ be a finite set of *vertices*, a multiset E consisting of $e \subseteq V$, $|e| = 2$ be *edges*, then we call $G = (V, E)$ a *graph*. We call G *normal*, if E is a set (i.e., there are no multiple edges in G).

A *tree* is a connected graph without cycles. For $V' \subseteq V$, let $G(V')$ denote a graph $(V', \{\{v, w\} \in E \,|\, v \in V', w \in V'\})$. Let $H = (V_H, E_H)$ be a graph. Then H is a *subgraph* of G, if $V_H \subseteq V, E_H \subseteq E$. Vertex $v \in V$ is an *articulation point* of G, if $G(V \setminus \{v\})$ is disconnected. G is *biconnected* if there are no articulation points in G. *Biconnected component* is a maximal subgraph of G without an articulation point.

The graph G is *planar* if it can be drawn on a plane without edge intersections. The corresponding drawing is referred to as *planar embedding* of G. When no ambiguity arises, we do not distinguish planar graph G from its embedding.

A set $E' \subseteq E$ is called a *perfect matching* (PM) of G, if edges of E' are disjoint and their union equals V. PM(G) denotes the set of all PMs of G. K_p denotes a complete (normal) graph on p vertices, and K_{33} denotes a utility graph. *Triple bond* is a graph of two vertices and three edges between them. *Multiple bond* is a graph of two vertices and at least three edges between them.

3. Problem Setup

Let $G = (V, E)$ be a normal graph, $|V| = N$. For each $v \in V$, define a random binary variable (a spin) $s_v \in \{-1, +1\}$, $S = (s_{v_1}, ..., s_{v_N})$. Subscript i will be used as shorthand for v_i, for brevity, thus $S = (s_1, ..., s_N)$. For each $e \in E$, define a *pairwise interaction* $J_e \in \mathbb{R}$. We associate assignment $X = (x_1, ..., x_N) \in \{-1, +1\}^N$ to vector S with probability as follows:

$$\mathbb{P}(S = X) = \frac{1}{Z} \exp\left(\sum_{e=\{v,w\} \in E} J_e x_v x_w \right), \quad (1)$$

where

$$Z = \sum_{X \in \{-1,+1\}^N} \exp\left(\sum_{e=\{v,w\} \in E} J_e x_v x_w \right).$$

The probability distribution (1) defines the so-called *zero-field (or pairwise) Ising model*, and Z is called the *partition function* (PF) of the zero-field Ising (ZFI) model. Notice that $\mathbb{P}(S = X) = \mathbb{P}(S = -X)$.

Given a ZFI model, our goal is to find Z (*inference*) and draw samples from the model efficiently.

4. Reducing Planar ZFI Model to PM Model

In this section, we consider a special case of planar graph G and introduce a transition from the ZFI model to the perfect matching (PM) model on a different planar graph.

We assume that the planar embedding of G is given (and if not, it can be found in $O(N)$ time (Boyer & Myrvold, 2004)). We follow (Schraudolph & Kamenetsky, 2009) in constructions discussed in this section.

4.1. Expanded Dual Graph

First, triangulate G by adding new edges e to E such that $J_e = 0$. (The triangulation does not change probabilities of the spin assignments.) Graph G is generated (use the same notation as for the original graph for convenience) and is biconnected with every face, including lying on the boundary, forming a triangle. Complexity of the triangulation procedure is $O(N)$, see (Schraudolph & Kamenetsky, 2009) for an example.

Second, construct a new graph, $G_F = (V_F, E_F)$, where each vertex f of V_F is a face of G, and there is an edge $e = \{f_1, f_2\}$ in E_F if and only if f_1 and f_2 share an edge in G. By construction, G_F is planar, and it is embedded in the same plane as G, so that each new edge $e = \{f_1, f_2\} \in E_F$ intersects the respective old edge. Call G_F a *dual graph* of G. Since G is triangulated, each $f \in V_F$ has degree 3 in G_F.

Third, obtain a planar graph $G^* = (V^*, E^*)$ and its embedding from G_F by substituting each $f \in V_F$ by a K_3 triangle so that each vertex of the triangle is incident to one edge, going outside the triangle (see Figure 1(a) for an illustration). Call G^* an *expanded dual graph* of G.

Newly introduced triangles of G^*, substituting G_F's vertices, are called *Fisher cities* (Fisher, 1966). We refer to edges outside triangles as *intercity edges* and denote their set as E_I^*. The set $E^* \setminus E_I^*$ of Fisher city edges is denoted as E_C^*. Notice that $e^* \in E_I^*$ intersects exactly one $e \in E$ and vice versa, which defines a bijection between E_I^* and E; denote it by $g : E_I^* \to E$. Observe also that $|E_I^*| = |E| \leq 3N - 6$, where N is the size of G. Moreover, E_I^* is a PM of (V^*, E^*), and thus $|V^*| = 2|E_I^*| = O(N)$. Since G^* is planar, one also finds that $|E^*| = O(N)$. Constructing G^* takes efforts of $O(N)$ complexity.

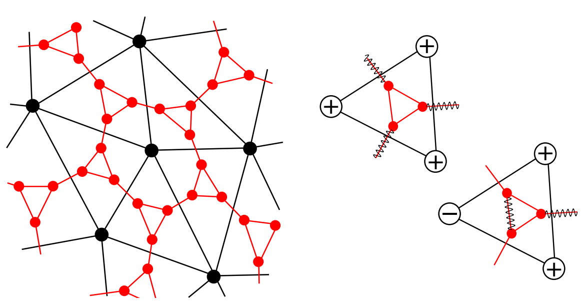

Figure 1. (a) A fragment of G's embedding after triangulation (black), expanded dual graph G^* (red). (b) Possible X configurations and corresponding $M(X)$ (wavy lines) on a single face of G. Rotation symmetric and reverse sign configurations are omitted.

4.2. Perfect Matching (PM) Model

For $X \in \{-1, +1\}^N$, let $I(X)$ be a set $\{e \in E_I^* \mid g(e) = \{v, w\}, x_v = x_w\}$. Each Fisher city is incident to an odd number of edges in $I(X)$. Thus, $I(X)$ can be uniquely completed to a PM by edges from E_C^*. Denote the resulting PM by $M(X) \in \text{PM}(G^*)$ (see Figure 1(b) for an illustration). Let $\mathcal{C}_+ = \{+1\} \times \{-1, +1\}^{N-1}$.

Lemma 1. *M is a bijection between $\mathcal{C}_+$ and PM(G^*).*

Define weights on G^* according to

$$\forall e^* \in E^* : c_{e^*} = \begin{cases} \exp(2J_{g(e^*)}), & e^* \in E_I^* \\ 1, & e^* \in E_C^* \end{cases}$$

Lemma 2. *For $E' \in PM(G^*)$ holds*

$$\mathbb{P}(M(S) = E') = \frac{1}{Z^*} \prod_{e^* \in E'} c_{e^*}, \tag{2}$$

where

$$Z^* = \sum_{E' \in PM(G^*)} \prod_{e^* \in E'} c_{e^*} = \frac{1}{2} Z \exp\left(\sum_{e \in E} J_e\right) \tag{3}$$

is the PF of the PM distribution (PM model) defined by (2).

Second transition of (3) reduces the Z computation to solve for Z^*. Furthermore, only two equiprobable spin configurations X' and $-X'$ (one of which is in $\mathcal{C}_+$) correspond to E', and they can be recovered from E' in $O(N)$ steps, thus resulting in the statement that one samples from (1) if sampling from (2) is known.

The PM model can be defined for an arbitrary graph $\hat{G} = (\hat{V}, \hat{E})$, $\hat{N} = |\hat{V}|$ with positive weights $c_e, e \in E'$, as a probability distribution over $\hat{M} \in \text{PM}(\hat{G})$: $\mathbb{P}(\hat{M}) \propto \prod_{e \in \hat{M}} c_e$.

Our subsequent derivations are based on the following:

Theorem 1. *Given the PM model defined on planar graph $\hat{G}$ of size $\hat{N}$ with positive edge weights $\{c_e\}$, one can find its partition function and sample from it in $O(\hat{N}^{\frac{3}{2}})$ time.*

Algorithms, constructively proving the theorem, are directly inferred from (Wilson, 1997; Thomas & Middleton, 2009), with minor changes/generalizations. Hence, we outline them in the supplementary material.

Corollary. *Inference and sampling of the PM model on G^* (and, hence, the ZFI model on G) take $O(N^{\frac{3}{2}})$ time.*

5. Dynamic Programming within Triconnected Components

Starting with this section, we present new results. We describe a general algorithm that allows us to perform inference and sampling from the ZFI model in the case where the triconnected components of the underlying graph are either planar or of $O(1)$ size.

5.1. Decomposition into Biconnected Components

Consider a ZFI model (1) over a normal graph $G = (V, E)$, $|V| = N$. If G is disconnected, then distribution (1) is decomposed into a product of terms associated with independent ZFI models over the connected components of G. Hence, we assume below, without loss of generality, that G is connected.

Let $G_1, ..., G_h$ be biconnected components of G. They form a tree if an edge is drawn between G_i and G_j whenever G_i and G_j share an articulation point. A simple reduction (see supplementary material) shows that inference and sampling on G are reduced to a series of inference and sampling on ZFI models induced by subgraphs $G_1, ..., G_h$.

Lemma 3. *Let $Z_1, ..., Z_h$ be partition functions of ZFI models induced by $G_1, ..., G_h$. Then,*

$$Z = 2^{-h} Z_1 Z_2 ... Z_h. \tag{4}$$

Sampling from $\mathbb{P}(S = X)$ is reduced to a series of sampling on $G_1, ..., G_h$ and $O(N)$ post-processing.

Observe also that all the articulation points and the biconnected components of G can be found in $O(N + |E|)$ steps (Hopcroft & Tarjan, 1973a). Therefore later on, we assume without loss of generality that G is biconnected.

5.2. Biconnected Graph as a Tree of Triconnected Components

In this subsection we follow (Hopcroft & Tarjan, 1973b; Gutwenger & Mutzel, 2001), see also (Mader, 2008) to define the tree of triconnected components. Following discussions of the previous subsection, one considers here a biconnected G.

Let $v, w \in G$. Divide E into equivalence classes $E_1, ..., E_k$ so that e_1, e_2 are in the same class if they lie on a common simple path that has v, w as endpoints. $E_1, ..., E_k$ are referred to as *separation classes*. If $k \geq 2$, then $\{v, w\}$ is a *separation pair* of G, unless (a) $k = 2$ and one of the classes is a single edge or (b) $k = 3$ and each class is a single edge. Graph G is called *triconnected* if it has no separation pairs.

Let $\{v, w\}$ be a separation pair in G with equivalence classes $E_1, ..., E_k$. Let $E' = \cup_{i=1}^{l} E_l, E'' = \cup_{i=l+1}^{k} E_l$ be such that $|E'| \geq 2$, $|E''| \geq 2$. Then, graphs $G_1 = (\cup_{e \in E'} e, E' \cup \{e_\mathcal{V}\}), G_2 = (\cup_{e \in E''} e, E'' \cup \{e_\mathcal{V}\})$ are called *split graphs* of G with respect to $\{v, w\}$, and $e_\mathcal{V}$ is a *virtual edge*, which is a new edge between v and w, identifying the split operation. Due to the addition of $e_\mathcal{V}$, G_1 and G_2 are not normal in general.

Split G into G_1 and G_2. Continue splitting G_1, G_2, and so on, recursively, until no further split operation is possible. The resulting graphs are *split components* of G. They can either be K_3 (triangles), triple bonds, or triconnected normal graphs.

Let $e_\mathcal{V}$ be a virtual edge. There are exactly two split components containing $e_\mathcal{V}$: $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$. Replacing G_1 and G_2 with $G' = (V_1 \cup V_2, (E_1 \cup E_2) \setminus \{e_\mathcal{V}\})$ is called *merging* G_1 and G_2. Do all possible mergings of the cycle graphs (starting from triangles), and then do all possible mergings of multiple bonds starting from triple bonds. Components of the resulting set are referred to as the *triconnected components* of G. We emphasize again that some graphs (i.e., cycles and bonds) in the set of triconnected components are not necessarily triconnected.

Lemma 4. *(Hopcroft & Tarjan, 1973b) Triconnected components are unique for G. Total number of edges within the triconnected components is at most* $3|E| - 6$.

Consider a graph T, where vertices (further referred to as *nodes* for disambiguation) are triconnected components, and there is an edge between a and b in T, when a and b share a (copied) virtual edge.

Lemma 5. *(Hopcroft & Tarjan, 1973b) T is a tree.*

Example. Figure 2 illustrates triconnected decomposition of a binconnected graph and intermediate steps towards it.

All triconnected components, and thus T, can be found in $O(N + |E|)$ steps (Hopcroft & Tarjan, 1973b; Gutwenger & Mutzel, 2001; Vo, 1983). Merging of two triconnected components is equivalent to contracting an edge in T (VI on Figure 2). After all possible mergings, G is recovered.

5.3. Inference via Dynamic Programming

Assume that there is a (small) number C bounding the size of each nonplanar triconnected component. In the following, we present a polynomial time algorithm that computes Z for a given (fixed) C.

First, one finds triconnected components of G and T in $O(N + |E|)$ steps. Choose a *root* node d in T. For any node $a \neq d$ in T, let the next node b (on a unique path from a to d) be a *parent* of a, and a be a *child* of b. Nodes, which do not have any children, are called *leaves*. For node a, let a *subtree* $T(a)$ denote a subgraph constructed from a, its children, grandchildren, and so on.

Our algorithm processes each node once. The node is only processed when all its children have been already processed, so a leaf is processed first and the root is processed last. Let $a = (V_a, E_a), N_a = |V_a|$ be a currently processed node. Let $G_a^T = (V_a^T, E_a^T)$ be a graph obtained by merging all nodes in $T(a)$. If a is a root, then $G_a^T = G$. Since the root is processed last, it outputs the desired PF, Z. Figure 3 provides a visualization of a node processing routine which is to be explained.

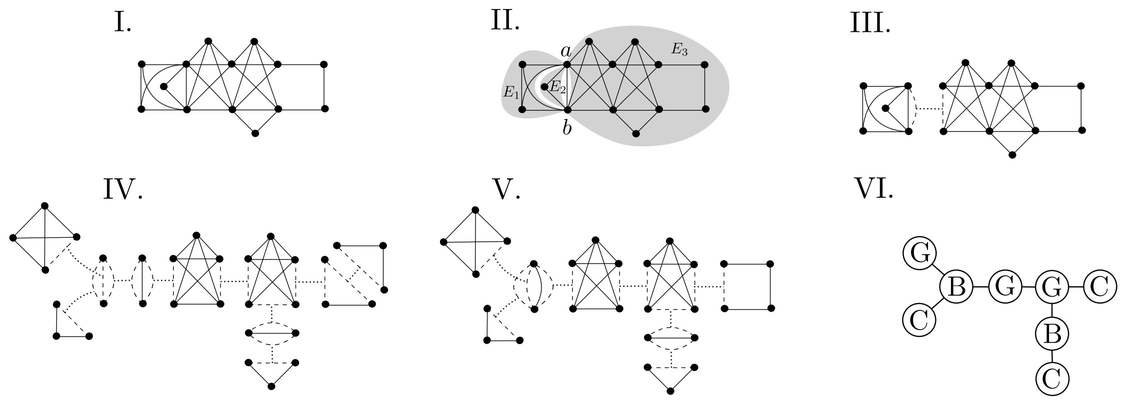

Figure 2. (I) An example biconnected graph G. (II) A separation pair $\{a, b\}$ of G and separation classes E_1, E_2, E_3 associated with $\{a, b\}$. (III) Result of split operation with $E' = E_1 \cup E_2, E'' = E_3$. Hereafter, dashed lines indicate virtual edges and dotted lines connect equivalent virtual edges in split graphs. (IV) Split components of G (non-unique). (V) Triconnected components of G. (VI) Triconnected component tree T of G; spacial alignment of V is preserved. "G," "B," and "C" are examples of the "triconnected graph," "multiple bond," and "cycle," respectively.

If a is not a root, let $e_{\mathcal{V}} = \{p, t\}$ be a virtual edge shared between a and its parent. The only virtual edge in G_a^T is $e_{\mathcal{V}}$, and G_a^T without $e_{\mathcal{V}}$ is a subgraph of G. Hence, pairwise interactions are defined for $E_a^T \setminus \{e_{\mathcal{V}}\}$. The result of node a's processing is a quantity.

$$\pi_a(x', x'') = \sum_{\substack{x_p = x', x_t = x'' \\ \forall u \in V_a^T \setminus e_{\mathcal{V}} : x_u = \pm 1}} \exp\left(\sum_{\substack{e = \{v, w\} \\ e \in E_a^T \setminus \{e_{\mathcal{V}}\}}} J_e x_v x_w \right),$$

where $x', x'' = \pm 1$. Notice that $\pi_a(+1, +1) = \pi_a(-1, -1)$, $\pi_a(+1, -1) = \pi_a(-1, +1)$, and hence $\pi_a(x', x'') = \pi_a(x'', x')$.

Processing nodes one by one we notice that the following cases are possible:

1. a **is a leaf**. Therefore, there is nothing to merge, and $a = G_a^T = (V_a, E_a)$. If a is nonplanar, find $\pi_a(\pm 1, \pm 1)$ by brute force enumeration, completed in $O(1)$ steps. If a is a multiple bond, $\pi_a(\pm 1, \pm 1)$ is found in $O(|E_a|)$ steps.

Assume now that node a is (or corresponds to) a planar, normal graph. Define $J_{e_{\mathcal{V}}} = 0$ and consider a ZFI model with the probability $\mathbb{P}_a(S_a = X_a)$ defined over graph a with $\{J_e \,|\, e \in E_a\}$ as pairwise interactions. Let Z_a be the PF of the ZFI model. In the remaining part of this case we will only work with this induced ZFI model, so that one can assume that nodes in V_a are ordered, $V_a = \{v_1, ..., v_{N_a}\}$, such that $v_1 = p, v_2 = t$. Then, one utilizes the notations $S_a = (s_1, ..., s_{N_a})$ and $X_a = (x_1, ..., x_{N_a}) \in \{-1, +1\}^{N_a}$ and derives

$$\pi_a(x', x'') = \sum_{X_a = (x', x'', \pm 1, ..., \pm 1)} \exp\left(\sum_{\substack{e = \{v, w\} \\ e \in E_a}} J_e x_v x_w \right)$$

$$= Z_a \mathbb{P}_a(x_1 = x', x_2 = x''). \tag{5}$$

Next, one triangulates a by adding enough edges with zero pairwise-interactions, similar to how it is done in Subsection 4.1. Assume that a is triangulated, and observe that the right-hand side of Eq. (5) is not affected. Construct $G^* = (V^*, E^*)$, which is an expanded dual graph of a with E_I^*, E_C^*, and g defined as in Subsection 4.1. Then, define mapping $M : \{-1, +1\}^{N_a} \to \text{PM}(G^*)$, weights c_{e^*}, and the PF Z^* as in 4.2. Denote $e_{\mathcal{V}}^* = g^{-1}(e_{\mathcal{V}})$.

According to the definition of M,

$$\begin{aligned} \mathbb{P}_a(x_1 = x_2) &= \mathbb{P}_a(e_{\mathcal{V}}^* \in M(S_a)) \\ &= \frac{1}{Z^*} \sum_{\substack{E' \in \text{PM}(G^*), \\ e_{\mathcal{V}}^* \in E'}} \prod_{e^* \in E'} c_{e^*}. \end{aligned} \tag{6}$$

Denote $G_{\mathcal{V}}^* = G^*(V^* \setminus e_{\mathcal{V}}^*)$. We continue the chain of relations/equalities (6) observing that

$$\{E' \in \text{PM}(G^*) \,|\, e_{\mathcal{V}}^* \in E'\} = \{E'' \cup \{e_{\mathcal{V}}^*\} \,|\, E'' \in \text{PM}(G_{\mathcal{V}}^*)\}.$$

Then one arrives at

$$\mathbb{P}_a(x_1 = x_2) = \frac{c_{e_{\mathcal{V}}^*}}{Z^*} \sum_{E'' \in \text{PM}(G_{\mathcal{V}}^*)} \prod_{e^* \in E''} c_{e^*} = \frac{c_{e_{\mathcal{V}}^*} Z_{\mathcal{V}}^*}{Z^*},$$

where $Z_{\mathcal{V}}^*$ is a PF of the PM model over $G_{\mathcal{V}}^*$. Compute Z^* and Z_a in $O(N_a^{\frac{3}{2}})$ steps, as described in Section 4. Since $G_{\mathcal{V}}^*$ is planar of size $O(N_a)$, $Z_{\mathcal{V}}^*$ can also be computed in $O(N_a^{\frac{3}{2}})$ steps, as Theorem 1 states. The following relations finalize computation of $\pi_a(\pm 1, \pm 1)$ in $O(N_a^{\frac{3}{2}})$ steps:

$$\pi_a(+1, +1) = \frac{Z_a}{2} \mathbb{P}_a(x_1 = x_2) = \frac{Z_a e_{\mathcal{V}}^* Z_{\mathcal{V}}^*}{2Z^*}$$

$$\pi_a(+1,-1)=\frac{Z_a}{2}\mathbb{P}_a(x_1\neq x_2)=\frac{Z_a}{2}-\pi_a(+1,+1).$$

2. a **is not a leaf, not a root**. Let $c_1,...,c_q$ be a's children, and $e^i_{\mathcal{V}}=\{p^i,t^i\}$ be a virtual edge shared between c_i and a, $1\leq i\leq q$. At this point, we already computed all $\pi_{c_i}(\pm1,\pm1)$. Each $\{p^i,t^i\}$ is a separation pair in G^T_a that splits it into $G^T_{c_i}$ and the rest of G^T_a, containing all $G^T_{c_j}$, $j\neq i$. Denote all virtual edges in a as $E_{\mathcal{V}}$, and then the following relation holds:

$$\pi_a(x',x'')=\sum_{\substack{x_p=x',x_t=x'',\\ \forall u\in V_a\setminus e_{\mathcal{V}}:x_u=\pm1}}\Bigg[\exp\Bigg(\sum_{\substack{e=\{v,w\}\\ e\in E_a\setminus E_{\mathcal{V}}}}J_e x_v x_w\Bigg)\cdot\prod_{i=1}^{q}\pi_{c_i}(x_{p^i},x_{t^i})\Bigg].\quad(7)$$

If a is (or corresponds to) a multiple bond, (7) is computed trivially in $O(|E_a|)$ steps. Hence, one assumes next that a is a normal graph.

Each $\pi_{c_i}(x',x'')$ is positive, and it essentially only depends on the product $x'x''$, that is, there exist such A_i,B_i that $\log\pi_{c_i}(x',x'')=A_i+B_ix'x''$. Using this relation, one rewrites (7) as

$$\pi_a(x',x'')=\sum_{\substack{x_p=x',x_t=x'',\\ \forall u\in V_a\setminus e_{\mathcal{V}}:x_u=\pm1}}\exp\Bigg(\sum_{\substack{e=\{v,w\}\\ e\in E_a\setminus E_{\mathcal{V}}}}J_e x_v x_w+\sum_{i=1}^{q}B_i x_{p^i}x_{t^i}\Bigg)\cdot\exp\Bigg(\sum_{i=1}^{q}A_i\Bigg).\quad(8)$$

Denote $J_{e_{\mathcal{V}}}=0$, $J_{e^i_{\mathcal{V}}}=B_i$ for each $1\leq i\leq q$. Then rewrite (8) as

$$\pi_a(x',x'')=\exp\Bigg(\sum_{i=1}^{q}A_i\Bigg)\cdot\sum_{\substack{x_p=x',x_t=x'',\\ \forall u\in V_a\setminus e_{\mathcal{V}}:x_u=\pm1}}\exp\Bigg(\sum_{e=\{v,w\}\in E_a}J_e x_v x_w\Bigg).\quad(9)$$

We compute (9) by brute force in $O(1)$ steps, if a is nonplanar. If a is normal planar, we once again consider a ZFI model with the probability $\mathbb{P}_a(S_a=X_a)$, defined over G_a, where the pairwise weights are $\{J_e\,|\,e\in E_a\}$, and Z_a is the respective PF. Then applying machinery from Case 1, one derives

$$\pi_a(x',x'')=\exp\Bigg(\sum_{i=1}^{q}A_i\Bigg)\cdot Z_a\mathbb{P}_a(x_p=x',x_t=x'')$$

in $O(N_a^{\frac{3}{2}})$ steps.

3. a **is a root**. Once again, let $c_1,...,c_q$ be children of a, $e^i_{\mathcal{V}}=\{p^i,t^i\}$ be a virtual edge shared between c_i and a, and $1\leq i\leq q$, $E_{\mathcal{V}}$ be the set of virtual edges in E_a (which a shares only with its children). Using considerations similar to those described while deriving Eq. (7), one arrives at

$$Z=\sum_{X\in\{-1,+1\}^N}\exp\Bigg(\sum_{e=\{v,w\}\in E}J_e x_v x_w\Bigg)=\sum_{\forall u\in V_a:x_u=\pm1}\Bigg[\exp\Bigg(\sum_{\substack{e=\{v,w\}\\ e\in E_a\setminus E_{\mathcal{V}}}}J_e x_v x_w\Bigg)\cdot\prod_{i=1}^{q}\pi_{c_i}(x_{p^i},x_{t^i})\Bigg].$$

Finally, one computes Z similarly to how the π values were derived in Case 2. It takes $O(|E_a|)$ steps if a is a multiple bond. Otherwise, one constructs a ZFI model and finds the PF over the respective graphs in either $O(1)$ steps, if the graph is nonplanar, or in $O(N_a^{\frac{3}{2}})$ steps, if a is normal planar.

5.4. Sampling via Dynamic Programming

The sampling algorithm, detailed below, follows naturally from the inference routine. Compute triconnected components of G in $O(N+|E|)$ steps. If all the triconnected components of G are multiple bonds, G should be a multiple bond itself, but G is normal. Therefore, there exists a component that is not a multiple bond; choose it as a root of T.

Use the inference routine (described in the previous Section) to compute Z. Now, do a backward pass through the tree, processing the root first, and then processing the node only when its parent has already been processed (Figure 4 visualizes the sampling algorithm).

Suppose a is a root and it is processed by now. Since a is not a multiple bond, it results in an Ising model, $\mathbb{P}_a(S_a=X_a)$. Draw a spin configuration X_a from this model. It will take $O(1)$ steps if a is nonplanar or $O(N_a^{\frac{3}{2}})$ steps if a is planar.

Suppose a is not a root. If a is a multiple bond, spin values were already assigned to its vertices (contained within the node/graph a). Otherwise, there exists a ZFI model $\mathbb{P}_a(S_a=X_a)$ already constructed at the inference stage. Following the notation of Subsection 5.3, one has to sample from $\mathbb{P}_a(S_a=X_a|s_p=x_p,s_t=x_t)$, since spins s_p and s_t are shared with the parent model and have already been drawn as x_p and x_t, respectively. If $x_p=x_t$, all valid X_a are such that $e^*_{\mathcal{V}}\in M(X_a)$, and the task is reduced to sampling PMs on $G^*_{\mathcal{V}}$. Otherwise, all valid X_a are such that $e^*_{\mathcal{V}}\notin M(X_a)$. Denote $\overline{G}^*_{\mathcal{V}}=(V^*,E^*\setminus\{e^*_{\mathcal{V}}\})$ and notice that

$$\{E'\in\text{PM}(G^*)\,|\,e^*_{\mathcal{V}}\notin E'\}=\text{PM}(\overline{G}^*_{\mathcal{V}}).$$

Therefore, the task is reduced to sampling PM over $\overline{G}^*_{\mathcal{V}}$.

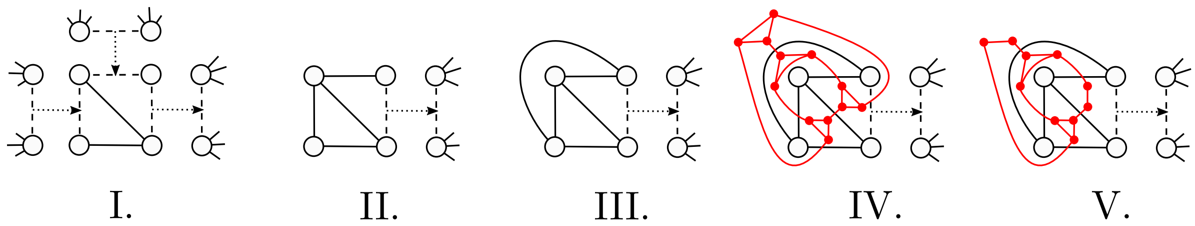

Figure 3. Inference. Illustration of a node processing. Arrow indicates a direction to the root. (I) Exemplary node a (subgraph in the center with one solid side edge, one solid diagonal edge, and solid dashed edges, marked according to the rules explained in the captions to Fig. 2), its (two) children and a parent. (II) Topology of the ZFI model defined on a. (III) Triangulated ZFI model. (IV) Expanded dual graph G^* of ZFI model (red). Computing PF Z^* of G^*'s PMs is a part of the inference processing of the node a. (V) $G^*_{\mathcal{V}}$ graph for a (red). Computing PF $Z^*_{\mathcal{V}}$ of $G^*_{\mathcal{V}}$ PMs is a part of the inference processing of node a, unless a is a root.

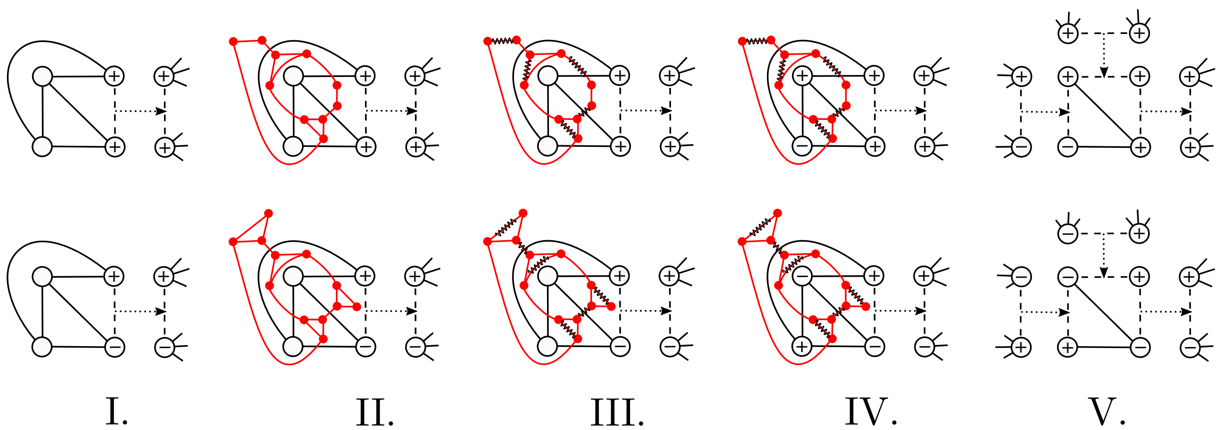

Figure 4. Sampling. Illustration of a node processing. General notations (arrows, children, parents, dashed and dotted lines) are consistent with the captions of Figs. 2,3. Assume that spin values at a's parent are already drawn (and consequently, spin values at $e_{\mathcal{V}}$ are drawn, too). The examples in the top line are for the case of equal spin values at $e_{\mathcal{V}}$, and the examples in the bottom line are for unequal spin values at $e_{\mathcal{V}}$. (I) Start with the triangulated ZFI model defined during inference (see Fig. 3). (II) Find either $G^*_{\mathcal{V}}$ (top, red) or $\overline{G}^*_{\mathcal{V}}$ (bottom, red) depending on spin values at $e_{\mathcal{V}}$. (III) Sample PM on $G^*_{\mathcal{V}}$ or $\overline{G}^*_{\mathcal{V}}$. (IV) Set spin values according to PM. (V) Propagate the spin values drawn along the virtual edges towards the child nodes.

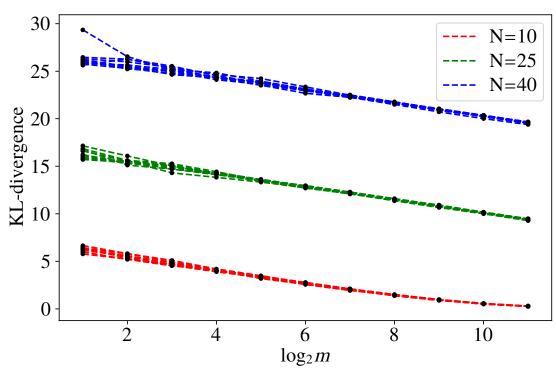

Figure 5. KL-distance of the model probability distribution compared with the empirical probability distribution. N, m are the model's size and the number of samples, respectively.

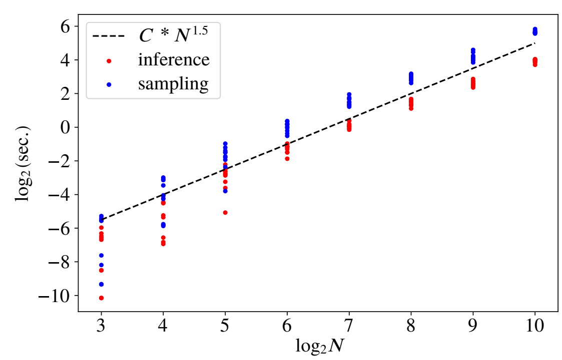

Figure 6. Execution time of inference (red dots) and sampling (blue dots) depending on N, shown on a logarithmic scale. Black line corresponds to $O(N^{\frac{3}{2}})$.

6. K_{33}-free Topology

6.1. ZFI Model over K_{33}-free Graphs

Consider the ZFI model (1) over a normal connected graph G. Let H be some graph. Then, H is a *minor* of G, if it is isomorphic to G's subgraph, in which some edges are contracted. (See (Diestel, 2006), Chapter 1.7, for a formal definition.)

G is K_{33}*-free*, if K_{33} is not a minor of G, that is, it cannot be derived from G's subgraph by contraction of some edges.

Let a biconnected G be decomposed into the tree of triconnected components. Then, the following lemma holds:

Lemma 6. *(Hall, 1943) Graph G is K_{33}-free if and only if its nonplanar triconnected components are exactly K_5.*

Therefore, if G is K_{33}-free, it satisfies all the conditions needed for efficient inference and sampling, described in Section 5. According to the lemma, the graph in Fig. 2 is K_{33}-free. The next statement expresses the main contribution of this manuscript.

Theorem 2. *If G is K_{33}-free, inference or sampling of (1) takes $O(N^{\frac{3}{2}})$ steps.*

We point out that the family of models for which the algorithm from Section 5 applies is broader than just K_{33}-free models. However, we focus on K_{33}-free graphs because they have a fortunate characterization in terms of a missing minor.

6.2. Discussion: Genus of K_{33}-free Graphs

A remarkable feature of K_{33}-free models is related to considerations addressing the graph's genus. *Genus* of a graph is a minimal genus (number of handles) of the orientable surface that the graph can be embedded into. Kasteleyn (Kasteleyn, 1963) has conjected that the complexity of evaluating the PF of a ZFI model embedded in a graph of genus g is exponential in g. The result was proven and detailed in (Regge & Zecchina, 2000; Gallucio & Loebl, 1999; Cimasoni & Reshetikhin, 2007; 2008). One naturally asks what are genera of graphs over which the ZFI models are tractable. The following statement relates biconnectivity and graph topology (genus):

Theorem 3. *(Battle et al., 1962) A graph's genus is a sum of its biconnected component genera.*

If a graph is not biconnected, its genus can be arbitrarily large, while inference and sampling may still be tractable in relation to the decomposition technique discussed in Subsection 5.1. Therefore, it becomes principally interesting to construct tractable biconnected models with large genus.

Lemma 7. *A biconnected K_{33}-free graph of size $5n$ can be of genus as big as n.*

From this we conclude that K_{33}-free graphs can't be tackled via the bounded-genus approach of (Regge & Zecchina, 2000; Gallucio & Loebl, 1999; Cimasoni & Reshetikhin, 2007; 2008). This justifies the novelty of our contribution.

7. Implementation and Tests

To test the correctness of inference, we generate random K_{33}-free models of a given size and then compare the value of PF computed in a brute force way (tractable for sufficiently small graphs) and by our algorithm. We simulate samples of sizes from $\{10, ..., 15\}$ (1000 samples per size) and verify that respective expressions coincide.

When testing sampling implementation, we take for granted that the produced samples do not correlate given that the sampling procedure (Section 5.4) accepts the Ising model as input and uses independent random number generation inside. The construction does not have any memory, therefore, it generates statistically independent samples. To test that the empirical distribution is approaching a theoretical one (in the limit of the infinite number of samples), we draw different numbers, m, of samples from a model of size N. Then we find Kullback-Leibler divergence between the probability distribution of the model (here we use our inference algorithm to compute the normalization, Z) and the empirical probability, obtained from samples. Fig. 5 shows that KL-divergence converges to zero as the sample size increases. Zero KL-divergence corresponds to equal distributions.

Finally, we simulate inference and sampling for random models of different size N and observe that the computational time (efforts) scales as $O(N^{\frac{3}{2}})$ (Fig. 6)[1].

8. Conclusion

In this manuscript, we compiled results that were scattered over the literature on $O(N^{\frac{3}{2}})$ sampling and inference in the Ising model over planar graphs. To the best of our knowledge, we are the first to present a complete and mathematically accurate description of the tight asymptotic bounds.

We generalized the planar results to a new class of zero-field Ising models over graphs not containing K_{33} as a minor. In this case, which is strictly more general than the planar case, we have shown that the complexity bounds for sampling and inference are the same as in the planar case. Along with the formal proof, we provided evidence of our algorithm's correctness and complexity through simulations.

[1] Implementation of the algorithms is available at https://github.com/ValeryTyumen/planar_ising.

Acknowledgements

This work was supported by the U.S. Department of Energy through the Los Alamos National Laboratory as part of LDRD and the DOE Grid Modernization Laboratory Consortium (GMLC). Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract No. 89233218CNA000001).

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