Valerii Likhosherstov¹, Yury Maximov^(1,2) and Michael Chertkov^(1,2)

¹ Skolkovo Institute of Science and Technology, Moscow, Russia

² Theoretical Division and Center for Nonlinear Studies,

Los Alamos National Laboratory, Los Alamos, NM, USA

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. To derive the algorithms, we use an equivalent linear transition to perfect matching counting and sampling on an expanded dual graph. 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

1 Introduction

Computing 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 [1]. Therefore, a question of interest becomes not to address the general case, but instead look after tractable families of Ising models. In the following, we review briefly tractability related to planar graphs and graphs embedded in surfaces of small genus.

Onsager [2] gave a closed-form solution for the partition function in the case of homogeneous interaction Ising model over infinite two-dimensional square grid without magnetic field. This result has opened up an exciting era of phase transition discoveries - arguably one of the most significant contributions in theoretical and mathematical physics of 20th century. Then, Kac and Ward [3] showed that in the case of a finite square lattice the problem of the partition function computation is reducible to a determinant. Kasteleyn [4] has 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 construction was also based on the so-called Pfaffian orientation which allows to count PMs by finding a single Pfaffian (or determinant) of a matrix. Fisher [5] simplified the Kasteleyn's construction such that the modified graph remained planar. Transition to PM is fruitful as it extends planar zero-field Ising model inference to models embedded on a torus [4] and, in fact, on any surface of small (orientable) genus g with a price of the additional, multiplicative and exponential in genus, 4^g , factor in the algorithm's running time [6].

The transition employed by Kac, Ward, Kasteleyn, and Fisher modifies partition function expression in such a way that the result is a sum over subgraphs with vertices of even degree. These subgraphs have no direct correspondence to spin configurations. Kasteleyn then made a modification of Ising model topology to switch to PM summation/counting. A parallel way of reducing the planar zero-field Ising model to a PM problem consists in constructing so-called expanded dual graph [7, 8, 9]. In this case, a dual graph is built - with faces of initial graph as vertices and connections indicating adjacency of faces. Then dual graph's vertices are substituted with Fisher's gadgets. This approach is more natural and interpretable since there is a one-toone correspondence between spin configurations and PMs on the expanded dual graph. An extra advantage of the approach is related to the fact that this reduction allows to develop an exact

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

efficient sampling. Based on linear algebra and planar separator theory [10], Wilson introduced algorithm [11] which allows to sample PMs over planar graphs in $O(N^{\frac{3}{2}})$ time. The algorithms were implemented in [12, 13] for the Ising model sampling, however, the implementation was limited to only the special case of a square lattice. In [12] 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. Therefore, incorporation of the bounded genus separators [14] generalizes $O(N^{\frac{3}{2}})$ sampling scheme to the case of arbitrary zero-field Ising models over graphs with a small genus. Notice, that imposing zero field condition is critical, as otherwise, the Ising model over a planar graph is NP-hard [8]. On the other hand, even in the case of zero magnetic field Ising models over general graphs are difficult. Indeed, another statement of [8] is that the zero-field Ising model over two-layer grid is NP-hard as well.

In this manuscript, we discuss tractability related to Ising model with zero magnetic fields over graphs more general than planar. Our construction is related to graphs characterized in terms of their excluded minor property. A graph G has a minor H, if H can be obtained from G by a series of edge contraction and vertex or edge deletion. According to the celebrated Robertson-Seymour result [15], families of graphs closed under the operation of evaluating minor can be characterized by a finite set of minimal minors they exclude. For planar graphs, this set is exactly $\{K_5, K_{33}\}$ (Wagner's theorem [16, 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_{33} minor or excluding the K_5 minor.

In this manuscript, we show that K_{33} -free zero-field Ising models are tractable in terms of inference and sampling and give 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. Notice that our construction is direct, i.e. it does not require the aforementioned construction of the extended dual graph. This direct feature of our derivation is principal. Indeed, the K_{33} -free graphs are comfortable to work with because their triconnected components are either planar or K_5 graphs [17]. This fact, in particular, makes possible to find Pfaffian orientation for counting or sampling PMs over such graphs efficiently [18]. However, a map from the Ising model over the K_{33} -free graphs to a PM model requires construction of the expanded dual graph which is no longer K_{33} -free. Therefore, the essence of our construction, instead, is to decompose inference task in Ising over K_{33} -free graph to a sequential dynamic programming evaluation over the planar or K_5 graphs in the spirit of [19]. 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 by an explicit example of a tractable problem over the graph with genus growing linearly with the graph size.

The manuscript is organized as follows. Sections 2 and 3, respectively, establish notations and pose the problems inference and sampling. Section 4 is a rigorous analysis of planar zero-field models. It is presented here both to provide a description of a $O(N^{\frac{3}{2}})$ inference and sampling method in planar models, which is to the best of our knowledge new, and also because 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 which are either planar or are 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 these in the planar case. Section 7 describes benchmarks justifying correctness and efficiency of our algorithm. We conclude the manuscript with conclusions and discussions of the path forward in Section 8.

2 Definitions and Notations

Let V be a finite set of vertices, a multiset $E \subseteq \{e \subseteq V : |e| = 2\}$ 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). We call G oriented, if each $e = \{v, w\} \in E$ is oriented as either $v \to w$ or $w \to v$. We call G weighted, if for each edge $e \in E$ there is a number c_e assigned to it.

A way to assign integer indices to V's elements, such that $V = \{v_1, ..., v_{|V|}\}$, is referred as V's numbering. We always imply that V has some fixed numbering. Edge $e \in E$ and a vertex $v \in V$ are *incident* if $v \in e$. A *degree* of v is a number of edges incident to it. $v \in V$ and $w \in V$ are *adjacent*, if $\{v, w\} \in E$.

Let $R = (v^1, v^2, ..., v^p)$ be a sequence of vertices, such that for each $1 \le i \le p-1$ v^i and v^{i+1} are adjacent. Then if all v^i are different, R is a *path* between v^1 and v^p . If all v^i except of v^1 and v^p are different, R is a *cycle* in G.

G is connected if there is a path between any pair of distinct vertices. A tree is a connected graph without cycles. For $V' \subseteq V$, let G(V') denote a graph $(V', \{\{v, w\} \in E \mid v \in V', w \in V'\})$. 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.

Let $P = \{p_v | v \in V\}$ be a set of distinct points on a plane, and $L = \{l_e | e \in E\}$ be a set of curves, such that for every $e = \{v, w\}$ curve l_e connects p_v and p_w . If curves from L only intersect in P, then a pair of P and L is called a *planar embedding* of G. If G has a planar embedding it is a *planar* graph. 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 normal graph on p vertices with all possible edges added. K_{33} is a complete bipartite graph on 6 vertices, divided in two equal groups (the utility graph). All possible edges are added to K_{33} , except of edges inside the group. *Triple bond* is a graph of two vertices and 3 edges between them. *Multiple bond* is a graph of two vertices and at least 3 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 a short-cut 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 the probability:

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

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 and draw samples from the model efficiently.

4 Planar Topology

In this section we introduce a polynomial algorithm, allowing to find Z and sample from (1) in a case when G is a planar graph. The complexity of both operations will be $O(N^{\frac{3}{2}})$.

We assume that the planar embedding of G is given (and if not it can be found in O(N) time) [20], and follow [9] in constructing the so-called expanded dual graph and then transiting to PM counting problem. To sample PMs, we use Wilson's algorithm [11] following and generalizing (to an arbitrary planar graph, and then beyond) the implementation ideas described in [12, 13] for regular planar square lattice.

4.1 Expanded Dual Graph

First of all, one triangulates G by adding new edges e to E such that $J_e = 0$ (obviously the triangulation does not change probabilities of the spin assignments), thus getting the graph G (use the same notion as for the original graph for convenience) which is biconnected with every face, including lying on the boundary, forming a triangle. Complexity of the triangulation procedure is O(N), see e.g. [9].

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 respective old edge (see Fig. 1a for an illustration). Call G_F a dual graph of G. Since Gis 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 triangle (see Figure 1b 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 [5]. 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 $|E^*| = O(N)$. To construct G^* takes efforts which are of O(N) complexity.



Figure 1: (a) A fragment of G's embedding after triangulation (black), embedding of dual graph G_F (red). (b) Same fragment of G (black) and expanded dual graph G^* (red). (c) 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 Counting Perfect Matchings

For $X \in \{-1, +1\}^N$ let I(X) be a set $\{e \in E_I^* | g(e) = \{v, w\}, x_v = x_w\}$. One can see that 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, $M(X) \in PM(G^*)$ (see Figure 1c for an illustration). Let $\mathcal{C}_+ = \{+1\} \times \{-1, +1\}^{N-1}$.

Lemma 1. M is a bijection between C_+ and $PM(G^*)$.

Proof. Let $E' \in PM(G^*)$. Call $e \in E$ saturated, if it intersects an edge from $E' \cap E_I^*$. Each Fisher city is incident to an odd number of edges in $E' \cap E_I^*$. Thus, each face of G has an even number of unsaturated edges. This property is preserved, when two faces/cycles are merged into one by evaluating respective symmetric difference. Therefore, one gets that any cycle in G has an even number of unsaturated edges.

For each *i* define $x_i := -1^{r_i}$, where r_i is the number of unsaturated edges on the path connecting v_1 and v_i . The definition is consistent due to aforementioned cycle property. Now for each $e = \{v, w\} \in E$, $x_v = x_w$ if and only if *e* is saturated. To conclude, we constructed *X* such that E' = M(X). Such *X* is unique, because parity of unsaturated edges on a path between v_1 and v_i uniquely determines relationship between x_1 and x_i , and x_1 is always +1.

Analogously, M is a bijection between $C_{-} = \{-1\} \times \{-1, +1\}^{N-1}$ and $PM(G^*)$. This follows from the definition of M and the aforementioned spin configuration symmetry fact, M(X) = M(-X).

Define weights on G^* according to

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

Let $E' \in \text{PM}(G^*)$ and $X' = (x'_1, ..., x'_N) \in \mathcal{C}_+, M(X') = E'$. Then

$$\mathbb{P}(M(S) = E') = 2\mathbb{P}(S = X')$$

$$= \frac{2}{Z} \exp\left(\sum_{e=\{v,w\}\in E} J_e x'_v x'_w\right)$$

$$= \frac{2}{Z} \exp\left(\sum_{e^*\in E'\cap E_I^*} 2J_{g(e^*)} - \sum_{e\in E} J_e\right)$$

$$= \frac{2}{Z} \exp\left(-\sum_{e\in E} J_e\right) \prod_{e^*\in E'\cap E_I^*} c_{e^*}$$

$$= \frac{2}{Z} \exp\left(-\sum_{e\in E} J_e\right) \prod_{e^*\in E'} c_{e^*}$$

$$= \frac{1}{Z^*} \prod_{e^*\in E'} c_{e^*}, \qquad (2)$$

where thus

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

is the PF of the perfect matching (PM) model just introduced. The second equality in the chain (2) follows from the (probability) normalization condition, $\sum_M \mathbb{E}'(M = E') = 1$.

Eq. (2) defines a distribution over $PM(G^*)$. Computing Z is equivalent to computing Z^* . Furthermore, since only two equiprobable spin configurations X' and -X' 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.

4.3 Pfaffian Orientation

Let $\hat{G} = (\hat{V}, \hat{E})$ be an oriented graph. Its cycle of even length (built on an even number of vertices) is said to be *odd-oriented*, if, when all edges along the cycle are traversed in any direction, an odd number of edges are directed along the traversal. An orientation of \hat{G} is called *Pfaffian*, if all cycles C, such that $\text{PM}(\hat{G}(\hat{V} - C)) \neq \emptyset$, are odd-oriented.

We will need G^* to contain a Pfaffian orientation, moreover the construction is easy.

Theorem 1. Pfaffian orientation of G^* can be constructed in $O(|V^*|) = O(N)$.

Proof. This theorem is proven constructively, see e.g. [11, 18], or [9], where the latter construction is based on specifics of the expanded dual graph.

Construct a skew-symmetric sparse matrix $K \in \mathbb{R}^{|V^*| \times |V^*|}$:

$$K_{ij} = \begin{cases} c_{e^*} & \{v_i^*, v_j^*\} \in E^*, v_i^* \to v_j^* \\ -c_{e^*} & \{v_i^*, v_j^*\} \in E^*, v_j^* \to v_i^* \\ 0 & \{v_i^*, v_j^*\} \notin E^* \end{cases}$$
(3)

The next result allows to compute, Z^* , and consequently, Z, in a polynomial time.

Theorem 2. det K > 0, $Z^* = \sqrt{\det K}$.

Proof. See, e.g., [11] or [4]. Notice, that the theorem applies to the PF of PM model over any planar graph, i.e. not only to the expanded dual graphs. \Box

4.4 Computing $\det K$

LU-decomposition of a matrix, A = LU, found via Gaussian decomposition, where L is a lowertriangular matrix with unit diagonals and U is an upper-triangular matrix, would be a standard way of computing det A, then equal to a product of the diagonal elements of U. However, this standard way of constructing the LU decomposition applies only if all A's leading principal submatrices are nonsingular. (See e.g. [21, Section 3.5] for detailed discussions.) And already the first, 1×1 , leading principal submatrix of K is zero/singular. Luckily, this difficulty can be resolved through the following construction. Take G^* 's arbitrary perfect matching $E' \in PM(G^*)$ - e.g. E_I^* . Modify ordering of vertices, $V^* = \{v_1^*, v_2^*, ..., v_{|V^*|}^*\}$, so that $E' = \{\{v_1^*, v_2^*\}, ..., \{v_{|V^*|-1}^*, v_{|V^*|}^*\}\}$. Build K according to the definition (3). Obtain \overline{K} from K by swapping column 1 with column 2, 3 with 4 and so on. This results in det $K = |\det \overline{K}|$, where the new \overline{K} is properly conditioned.

Lemma 2. \overline{K} 's leading principal submatrices are nonsingular.

Proof. The proof, presented in [11] for the case of unit weights c_{e^*} , generalizes to arbitrary positive c_{e^*} .

Notice, that in the general case (of a matrix represented in terms of a general graph) complexity of the LU-decomposition is cubic in the size of the matrix. Fortunately, *nested dissection* technique, discussed in the following subsection, allows to reduce complexity of computing Z to $O(N^{\frac{3}{2}})$.

4.5 Nested Dissection

Let $\hat{G} = (\hat{V}, \hat{E}), \hat{V} = \{\hat{v}_1, ..., \hat{v}_{\hat{N}}\}$ be a planar graph of size \hat{N} . Then partition P_1, P_2, P_3 of \hat{V} is a *separation* of \hat{G} , if for any $v \in P_1, w \in P_2$ it holds that $\{v, w\} \notin \hat{E}$. We refer to P_1, P_2 as the *parts*, and to P_3 as the *separator*.

Lipton and Tarjan (LT) [10] found an $O(\hat{N})$ algorithm, which finds a separation P_1, P_2, P_3 such that $\max(|P_1|, |P_2|) \leq \frac{2}{3}\hat{N}$ and $|P_3| \leq 2^{\frac{3}{2}}\sqrt{\hat{N}}$. The LT algorithm can be used to construct the so called *nested dissection ordering* of \hat{V} . The ordering is built recursively, by first placing vertices of P_1 , then P_2 and P_3 , and finally permuting indices of P_1 and P_2 recursively according to the ordering of $\hat{G}(P_1)$ and $\hat{G}(P_2)$. (See [22] for accurate description of details, definitions and analysis of the nested dissection ordering.) As shown in [22] the complexity of finding the nested dissection ordering is $O(\hat{N} \log \hat{N})$.

Let \hat{A} be a $\hat{N} \times \hat{N}$ matrix with a *sparsity pattern* of \hat{G} . That is, A_{ij} can be nonzero only if i = j or $\{\hat{v}_i, \hat{v}_j\} \in \hat{E}$.

Theorem 3. [22] If \hat{V} is ordered according to the nested dissection and A's leading principal submatrices are nonsingular, computing the LU-decomposition of A becomes a problem of the $O(N^{\frac{3}{2}})$ complexity.

Notice, however, that we cannot directly apply the Theorem to \overline{K} , because the sparsity pattern of K is asymmetric and does not correspond, in general, to any graph.

Let $G^{**} = (V^{**}, E^{**})$ be a planar graph, obtained from G^* , by contracting each edge in E', $|V^{**}| = |E'| = O(N)$. Find and fix a nested dissection ordering over V^{**} (it takes $O(N \log N)$ steps) and let the $\{v_1^*, v_2^*\}, \ldots, \{v_{|V^*|-1}^*, v_{|V^*|}^*\}$ enumeration of E' correspond to this ordering. Split K into 2×2 cells and consider the sparsity pattern of the nonzero cells. One observes that the resulting sparsity pattern coincides with the sparsity patterns of \overline{K} and G^{**} . Since LU-decomposition can be stated in the 2×2 block elimination form, its complexity is reduced down to $O(N^{\frac{3}{2}})$.

This concludes construction of an efficient inference algorithm for computing PF of a planar ZFI model.

4.6 Wilson's Sampling Algorithm

In [11] has constructed an algorithm which draws equiprobable configurations of perfect matchings over a planar graph in $O(N^{\frac{3}{2}})$ steps. The algorithm is based on the transformation from K to non-singular \overline{K} described above. Notice that a weighted version of the Wilson's algorithm, even though only for the case of a planar square lattice, was given in [12, 13].

To make the presentation within the manuscript self-consistent straightforward generalization of both the original Wilson algorithm (to non-equiprobable sampling) and of the Thomas-Middleton algorithm (to general planar graphs) are described in Appendix A.

5 Dynamic Programming within Triconnected Components

In this section we describe a general algorithm which allows to perform inference and sampling from the ZFI model in the case when the triconnected components of the underlying graph are either planar or of O(1) size. The approach is inspired by [19], where a dynamic programming over an auxiliary triconnected component tree was introduced to count perfect matchings. Here we extend the approach to ZFI. Moreover, from now on we work with the ZFI model directly bypassing mapping it to the perfect matching model followed so far in this manuscript.

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.

If G is not biconnected, it has at least two biconnected components. Clearly, each two biconnected components can only intersect at an articulation point and do not share edges. Moreover, a biconnected component containing a single articulation point should exist, as otherwise G is biconnected. Let v be this articulation point. Then there exists a separation $V_1, V_2, \{v\}$ of G, such that $G(V_2 \cup \{v\})$ is this component. Let $G_i = (\{v\} \cup V_i, E_i) = G(\{v\} \cup V_i), X_i$ be a sub-vector of X with indices $\{v\} \cup V_i$. Without loss of generality let $v_1 = v$. Let $\mathcal{C}_+^i = \{+1\} \times \{-1, +1\}^{|V_i|}$. Then one derives:

$$Z = 2 \sum_{X \in \mathcal{C}_{+}} \exp\left(\sum_{e=\{v,w\} \in E} J_e x_v x_w\right)$$
$$= 2 \sum_{X \in \mathcal{C}_{+}} \exp\left(\sum_{e=\{v,w\} \in E_1} J_e x_v x_w\right) \exp\left(\sum_{e=\{v,w\} \in E_2} J_e x_v x_w\right)$$
$$= 2 \sum_{X_1 \in \mathcal{C}_{+}^1} \exp\left(\sum_{e=\{v,w\} \in E_1} J_e x_v x_w\right) \sum_{X_2 \in \mathcal{C}_{+}^2} \exp\left(\sum_{e=\{v,w\} \in E_2} J_e x_v x_w\right)$$
$$= \frac{1}{2} Z_1 Z_2$$

where Z_i is the PF of the ZFI model induced by G_i . As far as sampling is concerned, let \mathbb{P}_i be a probability distribution induced by the *i*-th sub-model, S_i , be a sub-vector of S with indices $\{v\} \cup V_i$. Then, since $\mathbb{P}_2(s_1 = x_1) = \frac{1}{2}$:

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

= $2\frac{1}{Z_1} \exp\left(\sum_{e=\{v,w\} \in E_1} J_e x_v x_w\right) \frac{1}{Z_2} \exp\left(\sum_{e=\{v,w\} \in E_2} J_e x_v x_w\right)$
= $2\mathbb{P}_1(S_1 = X_1)\mathbb{P}_2(S_2 = X_2)$
= $\mathbb{P}_1(S_1 = X_1) \frac{\mathbb{P}_2(S_2 = X_2)}{\mathbb{P}_2(s_1 = x_1)}$
= $\mathbb{P}_1(S_1 = X_1)\mathbb{P}_2(S_2 = X_2|s_1 = x_1)$

Assume that a method for sampling S_i from \mathbb{P}_i is available. Then, draw X_1 by sampling S_1 from \mathbb{P}_1 . To sample S_2 conditional on $s_1 = x_1$ from \mathbb{P}_2 , draw $X'_2 = (x'_1, ...)$ from $\mathbb{P}_2(S_2 = X'_2)$. If $x'_1 = x_1$, then $X_2 = X'_2$, otherwise $X_2 = -X'_2$.

To conclude, one observes that inference and sampling in G are decomposed into inference and sampling in G_1 , which has fewer biconnected components, and in G_2 , which is biconnected. One continues this decomposition of G_2 into a biconnected component and the rest to reduce the problem, in the result, to inference and sampling over biconnected components.



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.

Observe also that all the articulation points and the biconnected components of G can be found in O(N + |E|) steps [23].

Therefore, later on, we assume, without loss of generality, that G is biconnected.

5.2 Biconnected Component as a Tree of Triconnected Components

In this subsection we follow [24, 25], see also [26], 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 path which can have only v, w as endpoints. $E_1, ..., E_k$ are referred to as separation classes. If $k \ge 2$, 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 $E' = \bigcup_{i=1}^l E_l, E'' = \bigcup_{i=l+1}^k E_l$ be such that $|E'| \ge 2$, $|E''| \ge 2$. Then graphs $G_1 = (\bigcup_{e \in E'} e, E' \cup \{e_v\}), G_2 = (\bigcup_{e \in E''} e, E'' \cup \{e_v\})$ are called *split graphs* of G with respect to $\{v, w\}$, and e_v is a virtual edge - new edge between v and w, identifying the split operation. Due to addition of e_v, G_1, G_2 are not normal in general.

Split G into G_1, G_2 , and 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_v be a virtual edge. There are exactly two split components $G_1 = (V_1, E_1), G_2 = (V_2, E_2)$, containing e_v . Replacing G_1 and G_2 with $G' = (V_1 \cup V_2, (E_1 \cup E_2) \setminus \{e_v\})$ is called *merging* G_1 and G_2 . Do all possible mergings of the cycle graphs (starting from triangles), 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 3. [24] 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 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 4. [24] 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 [24, 25, 27]. Merging of two triconnected components is equivalent to contracting an edge in T (VI on Figure 2). After all possible mergings are done, 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 which computes Z for 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 a 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 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 to a node processing routine which is to be explained.

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

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

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. Then, 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 $O(2^C \times C^2) = O(1)$ steps. If *a* is a multiple bond, $\pi_a(\pm 1, \pm 1)$ is found in $O(|E_a|)$ steps.

Assume now that the node a is (corresponds to) a planar, normal graph. Define $J_{e_v} = 0$ and consider a ZFI model with the probability $\mathbb{P}_a(S_a = X_a)$ defined over graph a with $\{J_e \mid e \in E_a\}$ 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

$$\pi_{a}(x',x'') = \sum_{\substack{X_{a} \in \{x'\} \times \{x''\} \times \{-1,+1\}^{N_{a}-2} \\ = Z_{a} \mathbb{P}_{a}(x_{1} = x', x_{2} = x'')}} \exp\left(\sum_{e=\{v,w\} \in E_{a}} J_{e}x_{v}x_{w}\right)$$
(4)

Next, one triangulates, a, by adding enough of edges with zero pairwise-interactions, similar to how it is done in Subsection 4.1. Now assume that a is triangulated, and observe that the right hand side of the Eq. (4) is not affected. Construct $G^* = (V^*, E^*)$ - 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 $e_v^* = g^{-1}(e_v)$. According to the definition of M:

$$\mathbb{P}_{a}(x_{1} = x_{2}) = \mathbb{P}_{a}(e_{v}^{*} \in M(X_{a})) = \frac{1}{Z^{*}} \sum_{\substack{E' \in \mathrm{PM}(G^{*}), e^{*} \in E' \\ e_{v}^{*} \in E'}} \prod_{e^{*} \in E'} c_{e^{*}}$$
(5)

Denote $G_v^* = G^*(V^* \setminus e_v^*)$. We continue the chain of relations/equalities (5) observing that

$$\{E' \in \operatorname{PM}(G^*) \, | \, e_v^* \in E'\} = \{E'' \cup \{e_v^*\} \, | \, E'' \in \operatorname{PM}(G_v^*)\}.$$

Then one arrives at

$$\mathbb{P}_{a}(x_{1} = x_{2}) = \frac{c_{e_{v}^{*}}}{Z^{*}} \sum_{E'' \in \mathrm{PM}(G_{v}^{*})} \prod_{e^{*} \in E''} c_{e^{*}} = \frac{c_{e_{v}^{*}} Z_{v}^{*}}{Z^{*}},$$

where Z_v^* is a PF of the PM model over G_v^* . Compute Z^* and Z_a in $O(N_a^{\frac{3}{2}})$ steps, as described in Section 4. Since G_v^* is planar of size $O(N_a)$, Z_v^* can also be computed in $O(N_a^{\frac{3}{2}})$ steps in the same way as Z^* was computed in Section 4 (Notice that even though G_v^* is not an expanded dual graph, only the feature of planarity is essential for this computation). The following relations finalize computation of $\pi_a(\pm 1, \pm 1)$ in $O(N_a^{\frac{3}{2}})$ steps:

$$\pi_a(+1,+1) = \pi_a(-1,-1) = \frac{Z_a}{2} \mathbb{P}_a(x_1 = x_2) = \frac{Z_a e_v^* Z_v^*}{2Z^*}$$
$$\pi_a(+1,-1) = \pi_a(-1,+1) = \frac{Z_a}{2} \mathbb{P}_a(x_1 \neq x_2) = \frac{Z_a}{2} - \pi_a(+1,+1)$$

End of Case 1.

2. *a* is not a leaf, not a root. Let $c_1, ..., c_q$ be *a*'s children, and $e_v^i = \{p^i, t^i\}$ be a virtual edge shared between c_i and $a, 1 \le i \le q$. At this point we have computed already all $\pi_{c_i}(\pm 1, \pm 1)$. Each $\{p^i, t^i\}$ is a separation pair in G_a^T which splits it into $G_{c_i}^T$ and the rest of G_a^T , containing all $G_{c_j}^T, j \ne i$. Denote all virtual edges in *a* as E_v , then the following relation holds:

$$\pi_{a}(x',x'') = \sum_{\substack{x_{p}=x',x_{t}=x'',\\\forall u\in V_{a}\setminus e_{v}:x_{u}=\pm 1}} \left[\exp\left(\sum_{\substack{e=\{v,w\}\\e\in E_{a}\setminus E_{v}}} J_{e}x_{v}x_{w}\right) \prod_{i=1}^{q} \pi_{c_{i}}(x_{p^{i}},x_{t^{i}}) \right]$$
(6)

If a is (corresponds to) a multiple bond, (6) 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 depends only on product x'x'' – i.e. there exist such A_i, B_i that $\log \pi_{c_i}(x', x'') = A_i + B_i x' x''$. Using this relation one rewrites (6) as

$$\pi_{a}(x',x'') = \sum_{\substack{x_{p}=x',x_{t}=x'',\\\forall u\in V_{a}\setminus e_{v}:x_{u}=\pm 1}} \exp\left(\sum_{\substack{e=\{v,w\}\\e\in E_{a}\setminus E_{v}}} J_{e}x_{v}x_{w} + \sum_{i=1}^{q} B_{i}x_{p^{i}}x_{t^{i}}\right) \cdot \exp\left(\sum_{i=1}^{q} A_{i}\right).$$
(7)

Denote $J_{e_v} = 0$, $J_{e_v^i} = B_i$ for each $1 \le i \le q$. Then rewrite (7) as

$$\pi_{a}(x',x'') = \exp\left(\sum_{i=1}^{q} A_{i}\right) \cdot \sum_{\substack{x_{p}=x', x_{t}=x'', \\ \forall u \in V_{a} \setminus e_{v}: x_{u}=\pm 1}} \exp\left(\sum_{e=\{v,w\} \in E_{a}} J_{e}x_{v}x_{w}\right)$$
(8)

We compute (8) by brute force in $O(2^C \times C^2) = O(1)$ steps, if *a* is nonplanar. If *a* is normal planar, we consider, once again, 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

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

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

End of Case 2.

3. *a* is a root. Once again, let $c_1, ..., c_q$ be children of $a, e_v^i = \{p^i, t^i\}$ be a virtual edge shared between c_i and $a, 1 \le i \le q$, E_v be the set of virtual edges in E_a (which *a* shares only with its children). Using considerations similar to the one already described while deriving Eq. (6), one arrives at

$$Z = \sum_{X \in \{-1,+1\}^N} \exp\left(\sum_{e=\{v,w\} \in E} J_e x_v x_w\right)$$
$$= \sum_{X \in \{-1,+1\}^N} \left[\exp\left(\sum_{\substack{e=\{v,w\}\\e \in E_a \mid E_v}} J_e x_v x_w\right) \prod_{i=1}^q \pi_{c_i}(x_{p^i}, x_{t^i})\right]$$

Finally, one computes Z in a way similar 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 ZFI model and find PF over the respective graphs in either $O(2^C \times C^2) = O(1)$ steps, if the graph is nonplanar, or in $O(N_a^{\frac{3}{2}})$ steps if a is normal planar.

End of Case 3.

5.4 Sampling via Dynamic Programming

Sampling algorithm, detailed below, follows naturally from the inference routine just detailed in the preceding subsection.

Compute triconnected components of G (and T) 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, which 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 the 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 $O(2^C \times C^2) = O(1)$ if *a* is nonplanar, or $O(N_a^{\frac{3}{2}})$ 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, s_t are shared with 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 $e_v^* \in M(X_a)$ and the task is reduced to sampling perfect matchings on G_v^* . Otherwise all valid X_a are such that $e_v^* \notin M(X_a)$. Denote $\overline{G}_v^* = (V^*, E^* \setminus \{e_v^*\})$ and notice that

$$\{E' \in \mathrm{PM}(G^*) \,|\, e_v^* \notin E'\} = \mathrm{PM}(\overline{G}_v^*).$$

Therefore, the task is reduced to sampling PM over \overline{G}_v^* .

6 K_{33} -free Topology

6.1 Inference and Sampling in the Zero-field Ising Model over K_{33} -free Graphs

Consider 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 [16, Chapter 1.7] for a formal definition).



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 perfect matchings is a part of the inference processing of the node a. (V) G_v^* graph for a (red). Computing PF Z_v^* of G_v^* PMs is a part of the inference processing of the 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. Illustration of a node processing. Assume that spin values at a's parent are already drawn (and, consequently, spin values at e_v are drawn, too). The example above is for the case of equal spin values at e_v , and the one below is for unequal spin values at e_v . (I) Start with the triangulated ZFI model defined during inference (see Fig. 3). (II) Find either G_v^* (above, red) or \overline{G}_v^* (below, red) depending on spin values at e_v . (III) Sample PM on G_v^* or \overline{G}_v^* . (IV) Set spin values according to PM. (V) Propagate the spin values just drawn along the virtual edges towards the child nodes.

G is K_{33} -free, if K_{33} is not a minor of G, i.e. it cannot be derived from G's subgraph by contraction of some edges. Planar graphs are included in the K_{33} -free family of graphs. Therefore the question of interest becomes to generalize tractable inference and sampling in the ZFI model over a K_{33} -free graph. Even though K_{33} -free graphs are Pfaffian orientable (with the Pfaffian orientation computable in polynomial time) [18], expanded dual graph, introduced to map ZFI model over K_{33} -free graph to respective PM problem is not necessarily K_{33} -free. Therefore the latter is generally not Pfaffian-orientable.

Let a biconected G be decomposed into the tree of triconnected components, then the following lemma holds

Lemma 5 (Hall, 1943). [17] Graph G is K_{33} -free, if and only if its nonplanar triconnected components are exactly K_5 .

Remark. Lemma 5, complemented with O(N + |E|) decomposition of the original graph into triconnected components [24, 25, 27] and planarity check of the decomposition components [20], suggests an efficient algorithm for checking whether a given graph is K_{33} -free. However, Lemma 5 also describes a way to construct any (biconnected) K_{33} -free graph. Indeed, take a set of K_5 's and arbitrary triconnected planar graphs, then "glue" these graphs along edges into a tree-like structure (like graph on Fig. 2 (I) is obtained from decomposition on Fig. 2 (V)).

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

Proof. Since G is normal and minor-free, it holds that |E| = O(N) [28]. Find all biconnected components and for each construct a triconnected component tree in O(N + |E|) = O(N).

As described above, the time (number of steps) of inference or sampling is a sum of inference or sampling times of each triconnected component of G. Let the set of all G's triconnected components (that is, a union over all biconnected components) to consist of k_1 planar triconnected components of size $N_1, ..., N_{k_1}$ with $M_1^p, ..., M_{k_1}^p$ edges respectively, k_2 multiple bonds of $M_1^b, ..., M_{k_2}^b$ edges and

 $k_3 K_5$ graphs. Then the complexity of inference or sampling is $O(\sum_{i=1}^{k_1} N_i^{\frac{3}{2}} + \sum_{i=1}^{k_2} M_i^b + k_3)$. The edges of G are partitioned among biconnected components. Inside each biconnected component apply second part of Lemma 3 to obtain that $\sum_{i=1}^{k_1} M_i^p + \sum_{i=1}^{k_2} M_i^b + 10k_3 = O(|E|) = O(N)$. This gives that $\sum_{i=1}^{k_2} M_i^b + k_3 = O(N)$ and $\sum_{i=1}^{k_1} M_i^p = O(N)$. Since triconnected components are connected graphs, we get that $N_i = O(M_i^p)$ for all $1 \le i \le k_1$ and hence $\sum_{i=1}^{k_1} N_i = O(N).$ From convexity of $f(x) = x^{\frac{3}{2}}$ it follows that $\sum_{i=1}^{k_1} N_i^{\frac{3}{2}} = O(N^{\frac{3}{2}})$ and finally that $O(\sum_{i=1}^{k_1} N_i^{\frac{3}{2}} + \sum_{i=1}^{k_2} M_i^b + k_3) = O(N^{\frac{3}{2}}).$

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

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 which the graph can be embedded into. Kastelyan [4] has conjected that complexity of evaluating partition function of ZFI model embedded in a graph of genus g is exponential in g. The result was proven and detailed in [29, 6, 30, 31]. 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 5. [32] 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.

A simple example illustrates that genus of a biconnected K_{33} -free graph can grow linearly with its size. First, notice that K_5 is a nonplanar graph, but it can be embedded in toroid (Fig. 5a), therefore genus of the graph is unity. Consider a cycle of length 2n, enumerate edges in the order of cycle traversal from 1 to 2n. Attach K_5 graph to each odd edge of the cycle (see Fig. 5b). The resulting graph G is of size 5n, it is biconnected and K_{33} -free (see Figure 5c). Remove an arbitrary even edge from the cycle. It results in a graph whose biconnected components are $n K_5$ graphs and n edges, so its genus is n. Since edge removal can only decrease genus, we conclude that G's genus is at least n.

$\mathbf{7}$ Implementation

We implement statistical inference and sampling for both planar and K_{33} -free cases, the code is available on GitHub².

To test our implementation, we, first, generate a random K_{33} -free graph, and, then choose the Ising interactions at random. Then we compute PF and generate samples over the randomly generated ZFI model.

Random Graph Generation 7.1

As our derivations cover the most general case of planar and K_{33} -free graphs, we want to test them on graphs which are as general as possible. For that purpose, we adapt and randomize a construction suggested in remark under Lemma 5. Namely, one generates a set of K_5 's and random planar graphs, attaching them by edges to a tree-like structure. For simplicity, we slightly relax the

²https://github.com/ValeryTyumen/planar_ising



Figure 5: (a) K_5 's embedding on a toroid - glue sides with the same label together. (b) G - a "necklace" of $n K_5$ graphs. (c) G's triconnected components. Dashed lines are virtual edges and dotted lines identify identical virtual edges. Triconnected components consist of a cycle, triple bonds and K_5 graphs. Hence, by Lemma 5 G is K_{33} -free.

condition that random planar components should be triconnected (because it is not clear how to generate such graphs efficiently) and simply require the components to be biconnected. This can be interpreted as constructing T, where some neighbor planar nodes are merged (merging planar graphs results in another planar graph). We refer to such non-unique decomposition T' as partially merged. Inference and sampling algorithm suggested in Section 5 is applied with no changes to the partially merged decomposition. Our generation process consists of the following two steps.

1. Planar graph generation. This step accepts $N \ge 3$ as an input and generates a normal biconnected planar graph of size N along with its embedding on a plane. The details of the construction are as follows.

First, a random embedded tree is drawn iteratively. We start with a single vertex, on each iteration choose a random vertex of an already "grown" tree, and add a new vertex connected only to the chosen vertex. Items I-V in Fig. 6 illustrate this step.

Then we triangulate this tree by adding edges until the graph becomes biconnected and all faces are triangles, as in the Subsection 4.1 (VI in Figure 6). Next, to get a normal graph, we remove multiple edges possibly produced by triangulation (VII in Fig. 6). At this point the generation process is complete.

2. K_{33} -free graph generation. Here we take $N \geq 5$ as the input and generate a normal biconnected K_{33} -free graph G in a form of its partially merged decomposition T'. Namely, we generate a tree T' of graphs where each node is either a normal biconnected planar graph or K_5 , and every two adjacent graphs share a virtual edge.

The construction is greedy and is essentially a tree generation process from Step 1. We start with K_5 root and then iteratively create and attach new nodes. Let N' < N be a size of the already generated graph, N' = 5 at first. Notice, that when a node of size n is generated, it contributes n - 2 new vertices to G.

An elementary step of iteration here is as follows. If $N - N' \ge 3$, a coin is flipped and the type of new node is chosen - K_5 or planar. If N - N' < 3, K_5 cannot be added, so a planar type is chosen. If a planar node is added, its size is drawn uniformly in the range between 3 and N - N' + 2 and then the graph itself is drawn as described in Step 1. Then we attach a new node to a randomly chosen free edge of a randomly chosen node of T'. We repeat this process until G is of the desired size N. Fig. 7 illustrates the algorithm.

To obtain an Ising model from G, we sample pairwise interactions for each edge of G independently from $\mathcal{N}(0, 0.1^2)$.

Notice that the tractable Ising model generation procedure is designed in this section solely for the convenience of testing and it is not claimed to be sampling models of any particular practical interest (e.g. in statistical physics or computer science).



Figure 6: Steps of planar graph generation. I-V refers to random tree construction on a plane, VI is a triangulation of a tree, VII is a result after multiple edges removal.



Figure 7: Generation of K_{33} -free graph G and its partially merged decomposition T'. Starting with K_5 (I), new components are generated and attached to random free edges (II-V). VI is a result graph G obtained by merging all components in T'.

7.2 Tests of Inference and Sampling

To test 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 $\{10, ..., 15\}$ and verify that respective expressions coincide.

As far as sampling implementation is concerned, we take for granted that produced samples do not correlate, since sampling procedure (Section 5.4) accepts Ising model as input and uses independent random number generation inside. The construction does not have any memory, therefore generating statistically independent samples. To test that the empirical distribution is approaching 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. 8a shows that KLdivergence 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 to observe that the computational time (efforts) scales as $O(N^{\frac{3}{2}})$ (Fig. 8b).

8 Conclusions and Path Forward

In this manuscript we, first of all, have compiled together results, scattered over literature, on sampling and inference in the Ising models over planar graphs. We have aimed at providing a comprehensive, self-consistent description of the methodology/theory and also at describing details of an efficient, $O(N^{\frac{3}{2}})$ complexity, implementation. Following the classic literature on the subject, our derivations relied on transition from the Ising model to the perfect matching model over the expanded dual graph [7, 8, 9], with subsequent construction of the Pfaffian orientation [4], and



Figure 8: (a) KL-distance of the model probability distribution compared with the empirical probability distribution. N, m are the model's size and number of samples respectively. (b) Execution time of inference (red dots) and sampling (blue dots) depending on N, shown in the logarithmic scale. Black line corresponds to $O(N^{\frac{3}{2}})$.

application of the nested dissection method [22] to make computation of the resulting determinant efficient. We have adopted the Wilson's algorithm for sampling planar matchings in planar graphs. To the best of our knowledge, we are the first to present complete and mathematically accurate description of the tight asymptotic bounds for sampling and inference over general planar graphs.

Then we generalize the planar results to a new class of zero-field Ising models over graphs not containing K_{33} as a minor. In this, strictly more general than planar, case we have shown that the complexity bounds for sampling and inference are the same as in the planar case. To derive these results we have decomposed the K_{33} minor free model into a biconnected graph built from an auxiliary decomposition tree with triconnected components which are each either a planar graph or exactly K_5 . Then we find the partition function of the zero-field Ising model over the graph via greedy, dynamic programming, approach advancing sequentially from leaves to the root of the decomposition tree. Sampling is computed via a backward pass, drawing spins at a node conditionally to spins within its parent. All the statements made casually above (in this paragraph) are proven. We also presented an efficient implementation for both inference and sampling 3 . We verify our theory through experiments (a) comparing the theory results for the partition function with brute force computation when these are feasible (small graphs), (b) checking exactness of our sampling procedure by testing dependence of KL divergence between the exact probability distribution and empirical probability distribution represented by samples, on the system size and the number of samples, (c) verifying that the computational time for inference and sampling scales according to $O(N^{\frac{3}{2}})$.

We conclude discussing a number of future research directions which:

- The class of models considered in the manuscript can be extended even further towards K_{33} -free generalizations of (a) the so-called outerplanar graphs, which can then be used for approximate inference and efficient learning in the spirit of [33] and [34] respectively; and (b) graphs embedded in the surfaces of O(1) genus [29, 6, 30, 31].
- This manuscript was motivated by a larger task of using efficient inference and learning over the most general K_{33} -graphs for constructing more general (and thus, hopefully, more powerful) alternatives to traditional Neural Networks for efficient learning.

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³https://github.com/ValeryTyumen/planar_ising

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Appendix A Wilson's Algorithm

A.1 Structure of the Algorithm

Let $N^* = |V^*| \leq 6N - 12$. Wilson's algorithm first applies LT algorithm of [10] to find a separation P_1, P_2, P_3 of G^* $(\max(|P_1|, |P_2|) \leq \frac{2}{3}N^*, |P_3| \leq 2^{\frac{3}{2}}\sqrt{N^*})$. Then it iterates over $v^* \in P_3$ and for each v^* it draws an edge of a perfect matching M, saturating v^* . Then it appears that, given this intermediate result, drawing remaining edges of the perfect matching M may be split into two independent drawings over $G^*(P_1)$ and $G^*(P_2)$, respectively, and then the process is repeated recursively. It takes $O(N^*)$ steps to sample edges attached to P_3 at the first step of the recursion, therefore the overall complexity of the Wilson's algorithm is also $O(N^*) = O(N^{\frac{3}{2}})$.

Subsection A.2 introduces probabilities required to draw the aforementioned PM samples. Subsections A.3 and A.4 describe how to sample edges attached to the separator, while Subsection A.5 focuses on describing the recursion.

A.2 Drawing Perfect Matchings

Let $M \in PM(G^*)$ come from the distribution (2), and for some $Q \in E^*$ consider the probability of getting Q as a subset of M:

$$\mathbb{P}(Q \subseteq M) = \frac{1}{Z^*} \sum_{\substack{M' \in \mathrm{PM}(G^*) \\ Q \subseteq M'}} \left(\prod_{e^* \in M'} c_{e^*} \right)$$
$$= \frac{1}{Z^*} \left(\prod_{e^* \in Q} c_{e^*} \right) \cdot \sum_{\substack{M' \in \mathrm{PM}(G^*) \\ e^* \in M' \setminus Q}} \left(\prod_{e^* \in M' \setminus Q} c_{e^*} \right)$$
(9)

Let $V_Q^* = \bigcup_{e^* \in Q} e^*$ and $G_{\setminus Q}^* = G^*(V^* \setminus V_Q^*)$. Then the set $\{M' \setminus Q \mid M' \in \text{PM}(G^*)\}$ coincides with $PM(G^*_{\setminus O})$. This yields the following expression

$$\mathbb{P}(Q \subseteq M) = \frac{Z^*_{\backslash Q}}{Z^*} \left(\prod_{e^* \in Q} c_{e^*}\right)$$

where

$$Z^*_{\backslash Q} = \sum_{M'' \in \mathrm{PM}(G^*_{\backslash Q})} \left(\prod_{e^* \in M''} c_{e^*}\right)$$

is a PF of the distribution of $PM(G_{\backslash Q}^*)$ induced by the edge weights c_{e^*} . For a square matrix A let $A_{c_1,...,c_l}^{r_1,...,r_l}$ denote the matrix obtained by deleting rows $r_1,...,r_l$ and columns $c_1,...,c_l$ from A. Let $[A]_{c_1,...,c_l}^{r_1,...,r_l}$ be obtained by leaving only rows $r_1,...,r_l$ and columns $c_1, ..., c_l$ of A and placing them in this order.

Now let $V_Q^* = \{v_{i_1}^*, ..., v_{i_r}^*\}, i_1 < ... < i_r$. A simple check demonstrates that deleting vertex from a graph preserves the Pfaffian orientation. By induction this holds for any number of vertices deleted. From that it follows that $K_{i_1,\ldots,i_r}^{i_1,\ldots,i_r}$ is a Kasteleyn matrix for $G^*_{\backslash Q}$ and then

$$Z^*_{\backslash Q} = \operatorname{Pf} K^{i_1, \dots, i_r}_{i_1, \dots, i_r} = \sqrt{\det K^{i_1, \dots, i_r}_{i_1, \dots, i_r}}$$

resulting in

$$\mathbb{P}(Q \subseteq M) = \sqrt{\frac{\det K_{i_1,\dots,i_r}^{i_1,\dots,i_r}}{\det K}} \cdot \left(\prod_{e^* \in Q} c_{e^*}\right)$$

Straightforward linear algebra transformations, described in [11], suggest that if A is nonsingular, then

$$\frac{\det A_{c_1,\dots,c_l}^{r_1,\dots,r_l}}{\det A} = \pm \det[A^{-1}]_{r_1,\dots,r_l}^{c_1,\dots,c_l}$$

This observation allows us to express probability (9) as

$$\mathbb{P}(Q \subseteq M) = \sqrt{|\det[K^{-1}]_{i_1,\dots,i_r}^{i_1,\dots,i_r}|} \cdot \left(\prod_{e^* \in Q} c_{e^*}\right)$$

Now we are in the position to describe the first step of the Wilson's recursion.

Step 1: Computing Lower-Right Submatrix of \overline{K}^{-1} A.3

Find a separation P_1, P_2, P_3 of G^* of G^* . The goal is to sample an edge from every $v^* \in P_3$.

Let T be a set of vertices from P_3 and their neighbors, then $|T| \leq 3|P_3|$ because each vertex in G^* is of degree 3. Let $T^{**} \subseteq V^{**}$ be a set of the contracted edges (recall G^{**} definition from Subsection 4.5), containing at least one vertex from $T, |T^{**}| \leq |T|$. Then T^{**} is a separator of G^{**} such that

$$|T^{**}| \le |T^*| \le 3|P_3| \le 3 \cdot 2^{\frac{3}{2}} \sqrt{N^*} \le 3 \cdot 2^2 \sqrt{|V^{**}|}$$
(10)

where one uses that, $|V^{**}| = \frac{N^*}{2}$. Find a nested dissection ordering (Subsection 4.5) of V^{**} with T^{**} as a top-level separator. This is a correct nested dissection due to Eq. (10).

Utilizing this ordering, construct \overline{K} . Compute L and U - LU-decomposition of \overline{K} $(O(N^{*\frac{3}{2}}))$ time). Let $t = 2|T^{**}| \leq 3 \cdot 2^{\frac{5}{2}} \sqrt{N^*}$ and let \mathcal{I} be a shorthand notation for $(N^* - t + 1, ..., N^*)$. Using L and U, find $D = [\overline{K}^{-1}]_{\mathcal{I}}^{\mathcal{I}}$, which is a lower-right \overline{K}^{-1} 's submatrix of size $t \times t$.

It is straightforward to observe that the *i*-th column of D, d_i , satisfies

$$[L]_{\mathcal{I}}^{\mathcal{I}} \times \left([U]_{\mathcal{I}}^{\mathcal{I}} \times d_i \right) = e_i,$$

where e_i is a zero vector with unity at the *i*-th position. Therefore constructing D is reduced to solving 2t triangular systems, each of size $t \times t$, resulting in $O(t^3) = O(N^{*\frac{3}{2}})$ required steps.

A.4 Step 2: Sampling Edges in the Separator

Now, progressing iteratively, one finds $v^* \in P_3$ which is not yet paired and draw an edge emanating from it. Suppose that the edges, $e_1^* = \{v_{j_1}^*, v_{j_2}^*\}, \dots, e_k^* = \{v_{j_{2k-1}}^*, v_{j_{2k}}^*\}$, are already sampled. We assume that by this point we have also computed LU-decomposition $A_k = [K^{-1}]_{j_1,\dots,j_{2k}}^{j_1,\dots,j_{2k}} = L_k U_k$ and we will update it to A_{k+1} when the new edge is drawn. Then

$$\mathbb{P}(e_1^*, ..., e_k^* \in M) = \sqrt{|\det A_k|} \prod_{j=1}^k c_{e_j^*}$$
(11)

Next we choose j_{2k+1} so that $v_{j_{2k+1}}^*$ is not saturated yet. We iterate over $v_{j_{2k+1}}^*$'s neighbors considered as candidates for becoming $v_{j_{2k+2}}^*$. Let v_j^* to become the next candidate, denote $e_{k+1}^* = \{v_{j_{2k+1}}, v_j^*\}$. For $n \in \mathbb{N}$ let $\alpha(n) = n+1$ if n is odd and $\alpha(n) = n-1$ if n is even. Then the identity

$$K^{-1} = [\overline{K}^{-1}]^{\alpha(1),\alpha(2),\dots,\alpha(N^*)}_{1,2,\dots,N^*},$$
(12)

follows from the definition of \overline{K} . One deduces from Eq. (12)

$$A_{k+1} = [K^{-1}]_{j_1, \dots, j_{2k+1}, j}^{j_1, \dots, j_{2k+1}, j} = [\overline{K}^{-1}]_{j_1, \dots, j_{2k+1}, j}^{\alpha(j_1), \dots, \alpha(j_{2k+1}), \alpha(j)}$$

Constructing T^{**} one has $j_1, ..., j_{2k+1}, j, \alpha(j_1), ..., \alpha(j_{2k+1}), \alpha(j) > N^* - t$. It means that A_{k+1} is a submatrix of D with permuted rows and columns, hence A_{k+1} is known.

We further observe that

$$A_{k+1} = \begin{bmatrix} A_k & y \\ r & d \end{bmatrix} = \begin{bmatrix} L_k & 0 \\ R & 1 \end{bmatrix} \begin{bmatrix} U_k & Y \\ 0 & z \end{bmatrix} = L_{k+1}U_{k+1}$$

Therefore to update L_{k+1} and U_{k+1} , one just solves the triangular system of equations $RU_k = r$ and $L_kY = y$, where R^{\top}, r^{\top}, Y, y are of size $2k \times 2$ (this is done in $O(k^2)$ steps), and then compute z = d - RY which is of the size 2×2 , then set, $u = \det z$.

The probability to pair $v_{j_{2k+1}}^*$ and v_j^* is

$$\begin{split} \mathbb{P}(e_{k+1}^* \in M \,|\, e_1^*, ..., e_k^* \in M) &= \frac{\mathbb{P}(e_1^*, ..., e_{k+1}^* \in M)}{\mathbb{P}(e_1^*, ..., e_k^* \in M)} \\ &= \frac{\sqrt{|\det A_{k+1}|} \prod_{j=1}^{k-1} c_{e_j^*}}{\sqrt{|\det A_k|} \prod_{j=1}^k c_{e_j^*}} \\ &= \frac{c_{e_{k+1}^*} \sqrt{|u|| \det A_k|}}{\sqrt{|\det A_k|}} \\ &= c_{e_{k+1}^*} \sqrt{|u|} \end{split}$$

Therefore maintaining U_{k+1} allows us to compute the required probability and draw a new edge from $v_{j_{2k+1}}$. By construction of G^* , $v_{j_{2k+1}}$ has only 3 neighbors, therefore the complexity of this step is $O(\sum_{k=1}^{|P_3|} k^2) = O(N^{*\frac{3}{2}})$ because $|P_3| \leq 2^{\frac{3}{2}}\sqrt{N^*}$.

A.5 Step 3: Recursion

Let $M_{sep} = \{e_1^*, e_2^*, ...\}$ be a set of edges drawn on the previous step, and V_{sep} be a set of vertices saturated by M_{sep} , $P_3 \subseteq V_{sep}$. Given M_{sep} , the task of sampling $M \in \text{PM}(G^*)$ such that $M_{sep} \subseteq M$ is reduced to sampling perfect matchings M_1 and M_2 over $G^*(P_1 \setminus V_{sep})$ and $G^*(P_2 \setminus V_{sep})$, respectively. Then $M = M_1 \cup M_2 \cup M_{sep}$ becomes the result of the perfect matching drawn from (2).

Even though only the first step of the Wilson's recursion was discussed so far, any further step in the recursion is done in exactly the same way with the only exception that vertex degrees may become less than 3, while in G^* they are exactly 3. Obviously, this does not change the iterative procedure and it also does not affect the complexity analysis.