Dimers and related combinatorial models of statistical mechanics

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MPRI course 2.10 Algorithmic Aspects of Combinatorics
Friday 13 December 2024

Plan

4. Dimer models on plane graphs: the Kasteleyn algorithm
   - The pfaffian
   - Pfaffian and dimers configurations

Reminders

Definition

Given a graph $G = (V, E)$, a dimer configuration on G is a subset C of E such that every vertex in V is incident to exactly one edge in C.

Remark: the number of vertices must be even for a dimer configuration to exist!

Our purpose is to address the following questions:

- given a finite graph G, how many dimer configurations does it admits?
- more generally, given edge weights $(w_e)_{e \in E}$, can we evaluate the dimer partition function

$$Z_{G,w} = \sum_{C} \prod_{e \in C} w_e$$

where the sum runs over all dimer configurations on G?

We have seen some specific methods working for specific graphs, and involving bijections with spanning trees or non intersecting lattice paths. Note that, in both cases, we ended up with the problem of evaluating the determinant of a certain matrix.

The Kasteleyn algorithm

We now describe a generic algorithm for counting dimer configurations of plane (and sometimes non-plane) graphs.

The algorithm relies on Kasteleyn's observation that, for graphs admitting certain suitable orientations, counting dimer configurations can be done by evaluating the determinant (or pfaffian) of a signed adjacency matrix.

For plane graphs, Kasteleyn show that these orientations always exist and can be constructed in linear time (in the size of the graph).

For a general graph, there may or may not exist such an orientation. This can be tested by a polynomial-time algorithm for bipartite graphs, but for other graphs the problem is still open to my knowledge.

The pfaffian

Let $M = (M_{ij})_{1 \le i,j \le n}$ be a $n \times n$ skew-symmetric matrix: $M_{ij} = -M_{ji}$.

- For n odd, its determinant is zero (why?).
- For n even, its determinant is a perfect square in the matrix entries:

$$
\begin{aligned}
n = 2: &\qquad \det M = (M_{12})^2, \\
n = 4: &\qquad \det M = (M_{12}M_{34} - M_{13}M_{24} + M_{14}M_{23})^2 \dots
\end{aligned}
$$

Theorem (Cayley, 1852)

Define the pfaffian of a $2m \times 2m$ skew-symmetric matrix by

$$\mathrm{pf}\, M = \frac{1}{2^m m!} \sum_{\sigma \in S_{2m}} \mathrm{sgn}(\sigma) \prod_{i=1}^{m} M_{\sigma(2i-1),\sigma(2i)}.$$

Then, we have

$$\det M = (\mathrm{pf}\, M)^2.$$

The pfaffian (continued)

An alternate expression for the pfaffian can be obtained as follows: let Π_m be the set of partitions of $\{1,\dots,2m\}$ into pairs. An element $\pi \in \Pi_m$ is called pairing and can be written as

$$\pi = \{\{\pi_1,\pi_2\},\{\pi_3,\pi_4\},\dots,\{\pi_{2m-1},\pi_{2m}\}\}$$

with

$$1 = \pi_1 < \pi_3 < \cdots < \pi_{2m-1}, \qquad \pi_{2i-1} < \pi_{2i}, \quad i = 1,\dots,m.$$

There are $(2m-1)!! = (2m-1)(2m-3)\cdots 3\cdot 1 = \frac{(2m)!}{2^m m!}$ such pairings.

A crossing of π is a pair of indices i,j such that $\pi_{2i-1} < \pi_{2j-1} < \pi_{2i} < \pi_{2j}$. The sign of π is

$$\mathrm{sgn}(\pi) = (-1)^{\#\{\text{crossings of } \pi\}}.$$

It is in fact the same as the signature of the permutation $i \mapsto \pi_i$. Then, we have

$$\mathrm{pf}\, M = \sum_{\pi\in\Pi_m} \mathrm{sgn}(\pi) \prod_{i=1}^{m} M_{\pi(2i-1),\pi(2i)}.$$

Proof of Cayley's theorem

Theorem (Cayley)

For M a $2m \times 2m$ skew-symmetric matrix we have

$$\det M = (\operatorname{pf} M)^2, \qquad \operatorname{pf} M := \sum_{\pi \in \Pi_m} \operatorname{sgn}(\pi) \prod_{i=1}^{m} M_{\pi(2i-1),\pi(2i)}.$$

The idea of the proof is as follows:

- expand $\det M$ as a sum over all permutations, and show by a sign-reversing involution that the contribution from permutations containing at least one cycle of odd length is zero,
- observe that there is a natural bijection between $\Pi_m \times \Pi_m$ and the set $E_{2m} \subset S_{2m}$ of permutations with all cycles of even lengths,
- check that this bijection is such that, for $(\pi, \pi') \mapsto \sigma$,

$$\operatorname{sgn}(\pi) \prod_{i=1}^{m} M_{\pi(2i-1),\pi(2i)} \times \operatorname{sgn}(\pi') \prod_{i=1}^{m} M_{\pi'(2i-1),\pi'(2i)} = \operatorname{sgn}(\sigma) \prod_{j=1}^{2m} M_{j,\sigma(j)}. \qquad \square$$

Pfaffian and dimer configurations

Now, let us make the connection with the enumeration of dimer configurations.

Let $G = (V, E)$ be a simple unoriented graph with vertex set $V = \{1, 2, \ldots, 2m\}$.
Let $(w_e)_{e \in E}$ be edge weights and A the corresponding weighted adjacency matrix.
Then, we have

$$Z_{G,w} := \sum_{C \text{ dimer config on } G} \left(\prod_{e \in C} w_e \right) = \sum_{\pi \in \Pi_m} \prod_{i=1}^{m} A_{\pi(2i-1)\pi(2i)}.$$

Indeed, a dimer configuration on G can be seen as a pairing $\pi \in \Pi_m$, with the property that $\pi(2i-1)$ and $\pi(2i)$ are adjacent in G for all i. Let us denote by Π_m^G the set of such pairings, and observe that pairings in $\Pi_m \setminus \Pi_m^G$ give a zero contribution to the right-hand side.

The quantity $\sum_{\pi \in \Pi_m} \prod_{i=1}^{m} A_{\pi(2i-1)\pi(2i)}$ is called the Hafnian of A, it looks very much like the pfaffian, but unfortunately does not have the same nice linear-algebraic properties.

A is symmetric and not skew-symmetric, so it does not make sense to talk about its pfaffian.

Pfaffian and dimer configurations (continued)

Given an orientation of the edges of G, let us define the signed adjacency matrix K by

$$K_{ij} = \begin{cases} w_e & \text{if there is an oriented edge } e \text{ from } i \text{ to } j, \\ -w_e & \text{if there is an oriented edge } e \text{ from } j \text{ to } i, \\ 0 & \text{otherwise.} \end{cases}$$

The signed adjacency matrix is skew-symmetric and its pfaffian is

$$\operatorname{pf} K := \sum_{\pi \in \Pi_m} \operatorname{sgn}(\pi) \prod_{i=1}^{m} K_{\pi(2i-1)\pi(2i)}.$$

Pfaffian orientations

Note that we have

$$\operatorname{sgn}(\pi) \prod_{i=1}^{m} K_{\pi(2i-1)\pi(2i)} = \pm \prod_{i=1}^{m} A_{\pi(2i-1)\pi(2i)}.$$

Indeed, the two quantities are either both equal to zero (if π does not correspond to a dimer configuration on G), or both nonzero. In this latter case, the sign on the right-hand side incorporates both $\operatorname{sgn}(\pi)$ and the sign involved when passing from K to A:

$$\frac{K_{\pi(2i-1)\pi(2i)}}{A_{\pi(2i-1)\pi(2i)}} = \begin{cases} +1 & \text{if the orientation goes from } \pi(2i-1) \text{ to } \pi(2i), \\ -1 & \text{if the orientation goes from } \pi(2i) \text{ to } \pi(2i-1). \end{cases}$$

We may rewrite this as $\operatorname{sgn}(\pi) \prod_{i=1}^{m} K_{\pi(2i-1)\pi(2i)} = \mathrm{ksgn}(\pi) \prod_{i=1}^{m} A_{\pi(2i-1)\pi(2i)}$ where

$$\mathrm{ksgn}(\pi) = (-1)^{\#\{\text{crossings of } \pi\} + \#\{i \text{ such that there is an edge oriented from } \pi(2i) \text{ to } \pi(2i-1)\}}.$$

This quantity depends implicitly on the orientation of the graph.

An orientation is said pfaffian if $\mathrm{ksgn}(\pi)$ is the same for all pairings $\pi \in \Pi_m^G$ (i.e. the pairings corresponding to dimer configurations on G).

Pfaffian orientations

Let us compare the two expressions obtained so far

$$Z_{G,w} = \sum_{\pi \in \Pi_m^G} \prod_{i=1}^{m} A_{\pi(2i-1)\pi(2i)},$$

$$\text{pf}\, K = \sum_{\pi \in \Pi_m^G} \mathrm{ksgn}(\pi) \prod_{i=1}^{m} A_{\pi(2i-1)\pi(2i)}.$$

When the orientation of the graph is pfaffian, that is when $\mathrm{ksgn}(\pi)$ is the same for all $\pi \in \Pi_m^G$, we have

$$Z_{G,w} = \pm\, \text{pf}\, K.$$

This is very interesting since the pfaffian, being the square root of the determinant, can be computed efficiently via linear algebra techniques.

But does such a "miraculous" pfaffian orientation exist? In the following we will see a more graph-theoretical characterization of pfaffian orientations, and then show that every plane graph admits at least one.

A characterization of Pfaffian orientations

Recall from the proof of Cayley's theorem that we have

$$\mathrm{sgn}(\pi)\prod_{i=1}^{m} K_{\pi(2i-1),\pi(2i)} \times \mathrm{sgn}(\pi')\prod_{i=1}^{m} K_{\pi'(2i-1),\pi'(2i)} = \mathrm{sgn}(\sigma)\prod_{j=1}^{2m} K_{j,\sigma(j)}$$

where $\sigma \in E_{2m}$ is the permutation with cycles of even length corresponding to $(\pi,\pi') \in \Pi_m^2$.

For $\pi,\pi' \in \Pi_m^G$, taking the sign of the above relation, we get

$$\mathrm{ksgn}(\pi)\mathrm{ksgn}(\pi') = (-1)^{\#\{\text{cycles of } \sigma\} + \#\{j=1,\ldots,2m \text{ such that there is an oriented edge from } \sigma(j) \text{ to } j\}}.$$

For a pfaffian orientation, we want this to be always equal to $+1$. A sufficient condition is that every cycle of σ is oddly-oriented, in the sense that it has an odd number of edges oriented in both directions. In fact, this is necessary if we want the relation to hold for any $\pi,\pi' \in \Pi_m^G$.

A characterization of Pfaffian orientations

We arrive at the following characterization of pfaffian orientations:

Definition (graph-theoretical version)

An orientation of a graph G is said pfaffian if every even central cycle is oddly oriented. Here:

- a cycle C is said even if it has an even number of edges,
- a cycle C is said central if the graph obtained from G by removing the vertices of C admits a dimer configuration,
- a cycle C is oddly oriented if it has an odd number of edges oriented in both directions.

(The even central cycles are precisely those arising as cycles of permutations σ obtained by superimposing two dimer configurations π, π'.)

Theorem

Let $G = (V, E)$ be a graph endowed with a pfaffian orientation. Let $w = (w_e)_{e \in E}$ be edge weights, and let K be the corresponding signed weighted adjacency matrix. Then, we have

$$Z_{G,w} = \pm \operatorname{pf} K = \pm\sqrt{\det K}.$$

Constructing a pfaffian orientation of a plane graph

Definition

An orientation of a plane graph G is said clockwise-odd if, around each bounded face of G, the number of edges oriented clockwise is odd.

It is straightforward to construct a clockwise-odd orientation: orient the edges of a spanning tree arbitrarily, then the other edges can be oriented in a unique manner.

Lemma

Let G be a plane graph endowed with a clockwise-odd orientation. Then, along each simple cycle C of G, the number of edges oriented clockwise has parity opposite to the number of vertices strictly in the interior of C.

The proof is based on Euler's relation.

Corollary

Every clockwise-odd orientation of a plane graph is pfaffian.