Dimers and related combinatorial models of statistical mechanics

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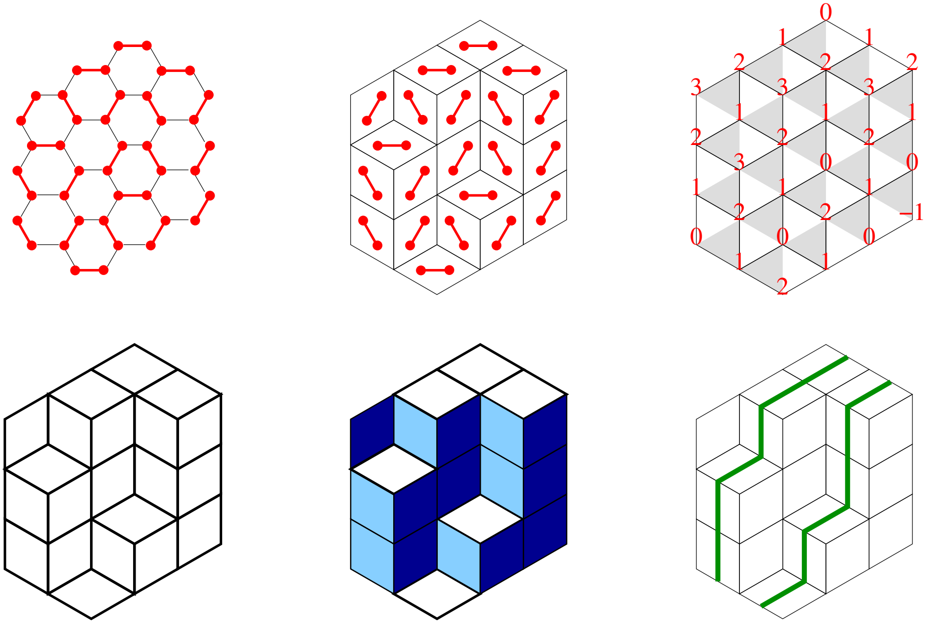
Plan

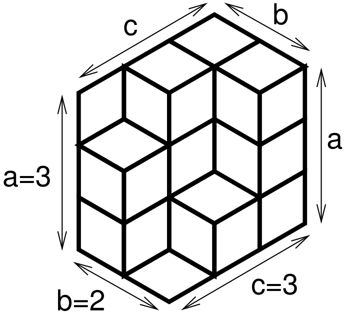
Dimers on the honeycomb lattice, lozenge tilings and other avatars



The MacMahon formula

Let us show how to enumerate dimer configurations on a hexagon-shaped portion of the honeycomb lattice, or equivalently the number of lozenge tilings of an hexagon.

Let us call $a \times b \times c$ hexagon a hexagon with angles 120° and integer side lengths a, b, c, a, b, c (when turning clockwise, note opposite sides have equal lengths).



Theorem (MacMahon, 1896)

The number of lozenge tilings of the $a \times b \times c$ hexagon is equal to

$$\mathcal{M}(a,b,c) = \prod_{i=1}^{a} \prod_{j=1}^{b} \prod_{k=1}^{c} \frac{i+j+k-1}{i+j+k-2}.$$

Riddle: how about hexagons whose opposite sides have unequal lengths?

The LGV lemma

Let $G = (V, E)$ be a directed acyclic graph and let $(w_e)_{e \in E}$ be weights for the edges. To an oriented path P on G, consisting of the edges $e_1, \ldots, e_k$, we associate a weight

$$w(P) = w_{e_1} \cdots w_{e_k}.$$

Fix $n \geq 1$ and two collections of vertices $u_1, \ldots, u_n$ (sources) and $v_1, \ldots, v_n$ (sinks). For any $i, j = 1, \ldots, n$, let M_{ij} be the sum of the weights of all paths from u_i to v_j.

For any permutation σ of size n, denote by $\mathcal{N}_\sigma$ the set of all n-tuples of non-intersecting paths $(P_1, \ldots, P_n)$ such that, for all $i = 1, \ldots, n$, P_i is a path from u_i to $v_{\sigma(i)}$. By non intersecting, we mean that P_i and P_j have no common vertex for any $i \neq j$.

Lemma (Lindström-Gessel-Viennot)

We have

$$\sum_{\sigma \in S_n} \mathrm{sgn}(\sigma) \sum_{(P_1, \ldots, P_n) \in \mathcal{N}_\sigma} w(P_1) \cdots w(P_n) = \det(M_{ij})_{1 \leq i,j \leq n}.$$

We often apply this lemma in the situation where, for planarity reasons, $\mathcal{N}_\sigma$ is empty unless σ is the identity permutation. Then the left-hand side reduces to a sum without signs.

Proof of the LGV lemma

Lemma (Lindström-Gessel-Viennot)

We have

$$\sum_{\sigma \in S_n} \operatorname{sgn}(\sigma) \sum_{(P_1,\dots,P_n)\in\mathcal{N}_\sigma} w(P_1)\cdots w(P_n) = \det(M_{ij})_{1\le i,j\le n}.$$

Proof: from the definition

$$M_{ij} := \sum_{P:u_i\to v_j} w(P)$$

an expansion of the determinant as a sum over permutations yields

$$\det(M_{ij})_{1\le i,j\le n} = \sum_{\sigma\in S_n} \operatorname{sgn}(\sigma) \sum_{(P_1,\dots,P_n)\in\mathcal{P}_\sigma} w(P_1)\cdots w(P_n)$$

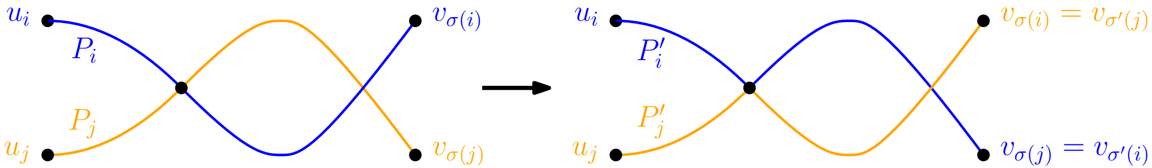
where $\mathcal{P}_\sigma$ is the set of all n-tuples of all (possibly intersecting) paths $(P_1,\dots,P_n)$ such that, for all $i=1,\dots,n$, P_i is a path from u_i to $v_{\sigma(i)}$. Thus, we need that intersecting tuples of paths give a zero total contribution to the sum.

Proof of the LGV lemma (continued)

Setting $\mathcal{I}_\sigma := \mathcal{P}_\sigma \setminus \mathcal{N}_\sigma$, we claim that

$$\sum_{\sigma \in S_n} \operatorname{sgn}(\sigma) \sum_{(P_1,\dots,P_n)\in\mathcal{I}_\sigma} w(P_1)\cdots w(P_n) = 0.$$

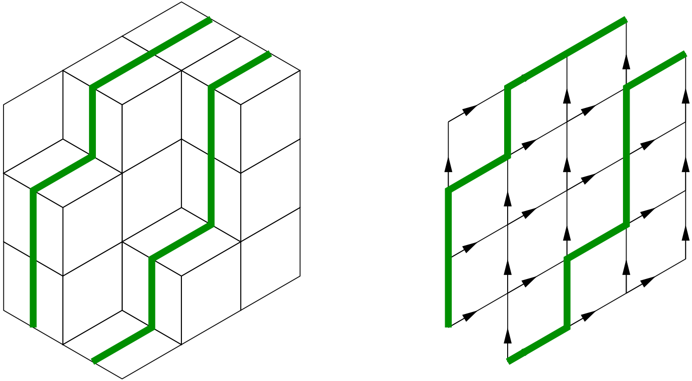
We define a sign-reversing involution on $\bigcup_{\sigma\in S_n}\mathcal{I}_\sigma$ as follows: given paths $(P_1,\dots,P_n)\in\mathcal{I}_\sigma$, we consider the smallest i such that P_i intersects another path, and then we consider the first intersection vertex along P_i, and the smallest $j > i$ such that P_j passes through that vertex. Doing a "switch" like this:



and leaving the other paths unchanged, we construct a n-tuple of paths in $\mathcal{I}_{\sigma'}$ with $\sigma' = \sigma \circ (ij)$. The edge weights are unchanged, but we have $\operatorname{sgn}(\sigma') = -\operatorname{sgn}(\sigma)$. We may check that the construction is involutive, and the claim follows. $\square$

Application to lozenge tilings

Lozenge tilings of the $a \times b \times c$ hexagon are in bijection with a-tuples of non-intersecting paths on the square lattice $\mathbb{Z}^2$ (with edges oriented up-right), going from the sources $u_i = (-i, i)$ to the sinks $v_j = (b-j, c+j)$, $i, j = 1, \ldots, a$.



By the LGV lemma their number is equal to $\det_{1\le i,j\le a} \binom{b+c}{c+j-i}$.

Actually, the number is unchanged if we make the paths start from the modified sources $u'_i = (-i, 1)$, $i = 1, \ldots, a$. The determinant $\det_{1\le i,j\le a} \binom{b+c+i-1}{c+j-1}$ is easier to evaluate.

Application to lozenge tilings (continued)

Indeed, we have

$$\mathcal{M}(a,b,c) = \det_{1\le i,j\le a} \frac{(b+c+i-1)!}{(c+j-1)!(b+i-j)!} = \det_{1\le i,j\le a} \frac{(b+c+i-1)!}{(b+i-1)!(c+j-1)!} \frac{(b+i-1)!}{(b+i-j)!}$$
$$= \prod_{i=1}^{a} \frac{(b+c+i-1)!}{(b+i-1)!(c+i-1)!} \det_{1\le i,j\le a} (b+i-1)(b+i-2)\cdots(b+i-j+1).$$

Note that $(b+i-1)(b+i-2)\cdots(b+i-j+1)$ is a monic polynomial of degree $j-1$ in i.

Proposition (Vandermonde determinant)

Let, for each $j=1,\ldots,a$, $q_j(X)$ be a monic polynomial of degree $j-1$ in the variable X. Then, given variables $X_1,\ldots,X_a$, we have

$$\det_{1\le i,j\le a} q_j(X_i) = \prod_{1\le i<j\le a} (X_j - X_i).$$

Proof: by columns manipulations, we can reduce to the case $q_j(X) = \prod_{i=1}^{j-1}(X-X_i)$ and the determinant is triangular. □

Application to lozenge tilings (continued)

By the Vandermonde determinant identity, we have

$$\det_{1\leq i,j\leq a}(b+i-1)(b+i-2)\cdots(b+i-j+1) = \prod_{1\leq i<j\leq a}(j-i) = \prod_{i=1}^{a}(i-1)!.$$

And hence, we have

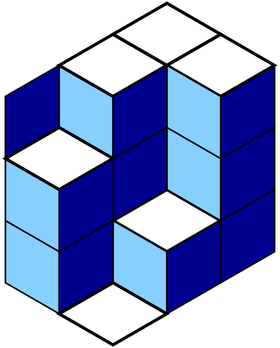
$$\begin{aligned}\mathcal{M}(a,b,c) &= \prod_{i=1}^{a}\frac{(b+c+i-1)!(i-1)!}{(b+i-1)!(c+i-1)!}\\ &= \prod_{i=1}^{a}\prod_{j=1}^{b}\frac{c+i+j-1}{i+j-1}\\ &= \prod_{i=1}^{a}\prod_{j=1}^{b}\prod_{k=1}^{c}\frac{i+j+k-1}{i+j+k-2}\end{aligned}$$

which is the MacMahon formula announced before.

Bonus

The MacMahon formula admits a "q-analogue". By this, we mean a formula depending on an extra variable q, recovering the previous formula for $q \to 1$. Usually, such formula involve the "q-integers"

$$[n]_q := \frac{1-q^n}{1-q} = 1 + q + q^2 + \cdots + q^{n-1}.$$



The volume is here 12.

To each lozenge tiling of the $a \times b \times c$ hexagon we may associate its "volume" (number of boxes when viewed in 3D).

Theorem (MacMahon, 1896)

The q^{volume} generating function of lozenge tilings of the $a \times b \times c$ hexagon is equal to

$$\mathcal{M}_q(a,b,c) = \prod_{i=1}^{a} \prod_{j=1}^{b} \prod_{k=1}^{c} \frac{1-q^{i+j+k-1}}{1-q^{i+j+k-2}}.$$

Bonus (continued)

This result may be again proved using the LGV lemma. In fact, inside the determinants to evaluate we just need to replace the binomial coefficients by their q-analogues:

$$\binom{n}{k}_q = \frac{(1-q^n)(1-q^{n-1})\cdots(1-q^{n-k+1})}{(1-q^k)(1-q^{k-1})\cdots(1-q)}.$$

Such q-binomial coefficients are actually polynomials in q, they satisfy the q-Pascal identity

$$\binom{n}{k}_q = q^k \binom{n-1}{k}_q + \binom{n-1}{k-1}_q$$

which shows that $\binom{n}{k}_q$ is the generating function of up-right paths on $\mathbb{Z}^2$ from $(0,0)$ to $(n-k,k)$ with a weight q^{area}. (Area is that of the region between the path and the x-axis.)

The q-binomial coefficients appear in the q-binomial theorem:

$$\prod_{i=0}^{n-1}(1+q^i z) = \sum_{k=0}^{n} q^{k(k-1)/2} \binom{n}{k}_q z^k.$$

Other applications

The method of counting lozenge tilings of a domain in the plane via the LGV lemma applies to many domain shapes other than the $a \times b \times c$ hexagon.

It is also possible to enumerate domino tilings of certain planar domains using a bijection with families of non-intersecting *Schröder* paths. Maybe we'll see some examples as an exercise.

An advantage of the LGV method is that the determinants to evaluate are smaller than those obtained via the Temperley/matrix-tree theorem approach or the generic Kasteleyn algorithm which we describe next.

Let us mention that there are many *methods* to evaluate the determinants that are encountered by the LGV approach, see e.g. the paper *Advanced determinant calculus* by C. Krattenthaler (1999), and more recent developments (Koutschan, Zeilberger...) using computer algebra.

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 $M = (M_{ij})_{1\leq i,j\leq n}$ 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:

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

Theorem (Cayley, 1852)

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

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

Then, we have

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

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

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

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 $(\pi, \pi') \mapsto \sigma$,

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

To be continued...

Next time we will see the connection with between these considerations and the dimer model.