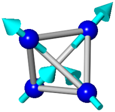

Cumulant expansion for counting Eulerian orientations

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joint work with Brendan D. McKay (ANU)
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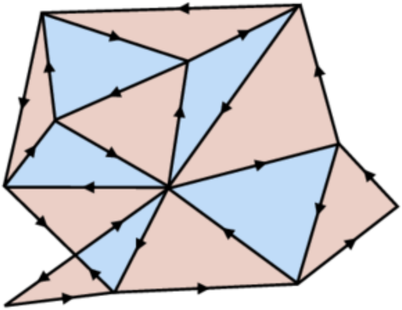
Talk structure

1. Introduction
2. Analytical approach (some not-very-old results)
3. Cumulant expansion (arXiv:2309.15473)
4. Residual entropy estimates (brand-new stuff)

Introduction

Definition

An *Eulerian orientation* is an orientation of the edges of a graph such that in-degree equals out-degree for each vertex.

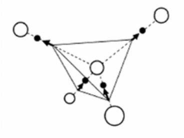


A graph admits an Eulerian orientations if and only if all degrees are even. However, counting such orientations is not easy!

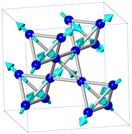
$\mathbf{EO}(\boldsymbol{G})$ denotes the number of Eulerian orientations in a graph $\boldsymbol{G}$.

Connection to statistical physics

[Pauling, 1935]: the hydrogen atoms in water ice are expected to remain disordered even at absolute zero. He introduced **"two-near, two-far" ice rule.**



EO(G) is equivalent to the crucial partition function in the **ice-type models** (ferroelectricity and spin ice). For planar graphs it reduces to the **six-vertex model.**



[Lieb, 1967] determined the asymptotics for the square ice:

$$\lim_{n\to\infty} \mathrm{EO}(L_n)^{\frac{1}{n}} = \frac{8\sqrt{3}}{9} \approx 1.540.$$

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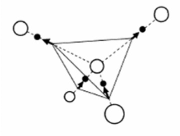

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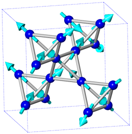

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The asymptotics for the 3D cubic ice is a **big open question** in the area.

Pauling's estimate

Assign orientation randomly for each edge. Let $\boldsymbol{X_i}$ denote the event that vertex $\boldsymbol{i}$ is "balanced". Then, $\mathbf{EO}(\boldsymbol{G}) = 2^{|\boldsymbol{E}(\boldsymbol{G})|}\,\mathbf{Pr}\left(\bigcap_{j=1}^{n} \boldsymbol{X_j}\right)$.

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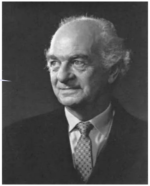
Let's pretend that they are independent!



$$\mathbf{EO}(G) \overset{?}{\approx} 2^{|E(G)|}\prod_{j=1}^{n}\mathbf{Pr}\left(X_j\right) = \frac{1}{2^{|E(G)|}}\prod_{j=1}^{n}\binom{d_j}{d_j/2}.$$

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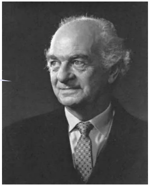

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You are being naive, Linus Pauling!

Regular tournaments

Theorem 1 (McKay, 1990)

For odd $n \to \infty$, we have $\mathbf{EO}(K_n) \sim \left(\frac{n}{e}\right)^{\frac{1}{2}} \left(\frac{2^{n+1}}{\pi n}\right)^{\frac{1}{2}(n-1)}$.

For $n = 5$, Theorem 1 gives ≈ 22.5. Pauling's estimate is $\left(\frac{3}{2}\right)^5 \approx 7.6$.

Asymptotically, Pauling's estimate is also not correct:

$$2^{-\frac{n(n-1)}{2}} \binom{n-1}{\frac{1}{2}(n-1)}^n \sim 2^{-\frac{n(n-1)}{2}} \left(\frac{2^{n-1} e^{\frac{1}{4(n-1)}}}{\sqrt{\frac{1}{2}\pi(n-1)}}\right)^n$$

$$\sim \mathbf{EO}(K_n)\, 2^{\frac{1}{2}} \pi^{-\frac{1}{2}} e^{-\frac{3}{4}} n^{-1}.$$

Analytical approach

Counting with integrals

First, observe

$$\mathbf{EO}(K_n) = [z_1^0 \cdots z_n^0] \prod_{j<k} \left(\frac{z_j}{z_k} + \frac{z_k}{z_j} \right).$$

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Using the Cauchy integral theorem, we get

$$\mathbf{EO}(K_n) = \frac{1}{(2\pi i)^n} \oint \cdots \oint \prod_{j<k} \left(\frac{z_j}{z_k} + \frac{z_k}{z_j} \right) dz_1 \ldots dz_n.$$

Setting contours to be unit circles, we get

$$\mathbf{EO}(K_n) = 2^{\frac{n(n-1)}{2}} \pi^{-n} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \prod_{j<k} \cos(\theta_j - \theta_k) d\theta.$$

Asymptotics of the integral

$$\mathrm{EO}(K_n) = 2^{\frac{n(n-1)}{2}} \pi^{-n} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \prod_{j<k} \cos(\theta_j - \theta_k) d\theta.$$

If all θ_j are approximately equal, we expand

$$\prod_{j<k} \cos(\theta_j - \theta_k) \sim \exp\left(-\tfrac{1}{2} \sum_{j<k} (\theta_j - \theta_k)^2 - \tfrac{1}{12} \sum_{j<k} (\theta_j - \theta_k)^4 \right).$$

Diagonalising the quadratic form, [McKay, 1990] shows

$$\int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \prod_{j<k} \cos(\theta_j - \theta_k) d\theta \sim \frac{2^{\frac{n-1}{2}} \pi^{\frac{n+1}{2}}}{n^{\frac{n-2}{2}}} e^{-1/2}.$$

Extension to general graphs

$$\mathrm{EO}(G) = 2^{|E(G)|}\pi^{-n}\int_{-\pi}^{\pi}\cdots\int_{-\pi}^{\pi}\prod_{jk\in G}\cos(\theta_j-\theta_k)d\theta.$$

$$\sim \frac{2^{|E(G)|}}{\sqrt{\det'(L)}}\left(\frac{2}{\pi}\right)^{(n-1)/2}\mathbb{E}e^{f_2(X_t)},$$

where X_t is a truncated singular Gaussian with density prop. to $e^{-\frac{1}{2}x^T Lx}$,

$$\theta^T L\theta := \sum_{jk\in G}(\theta_j-\theta_k)^2,$$

$$f_2(\theta) := -\frac{1}{12}\sum_{jk\in G}(\theta_j-\theta_k)^4.$$

From the Matrix Tree Theorem, we know that $\det'(L)$ is the number of spanning trees of G, which we denote by $t(G)$.

Two ideas, one additional assumption

Idea 1. McKay's integral estimate is equivalent to

$$\mathbb{E}e^{f_2(X_t)} \sim e^{\mathbb{E}f_2(X_t)} \sim e^{\mathbb{E}f_2(X)}.$$

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Idea 2. When $|\theta_1 - \theta_2|$ is large we need a lot of pairs j, k such that

$$|\cos(\theta_j - \theta_k)| < 1,$$

so the contribution of these θ to the integral is negligible. We can use short edge-disjoint paths from 1 to 2.

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Everything works out if $h(G) \geqslant \gamma n$ for some fixed γ, where

$$h(G) := \min_{|V| \leqslant n/2} \frac{|\partial_G(V)|}{|V|}.$$

A result from my PhD thesis

Theorem 2 (Isaev, Isaeva, 2013)

Suppose $h(G) \geqslant \gamma n$ and all degrees are even, then as $n \to \infty$

$$\mathrm{EO}(G) = \frac{2^{|E(G)|}}{\sqrt{t(G)}} \left(\frac{2}{\pi}\right)^{(n-1)/2} \exp\left(-\frac{1}{4}\sum_{jk \in G}\left(\frac{1}{d_j}+\frac{1}{d_k}\right)^2\right).$$

- For $G = K_n$, Theorem 2 reduced to Theorem 1 (McKay, 1990).
- $h(G) \geqslant \gamma n$ holds for asymptotically almost all dense graphs.
- In [Isaev, Iyer, McKay, 2020], we further extend Theorem 2 for graphs such that $h(G) \geqslant \gamma\Delta$, where $\Delta \geqslant n^{1/2+\varepsilon}$ is the maximal degree of G.

Cumulant expansion

Can we achieve a better precision?

$$\mathrm{EO}(G) = 2^{|E(G)|}\pi^{-n}\int_{-\pi}^{\pi}\cdots\int_{-\pi}^{\pi}\prod_{jk\in G}\cos(\theta_j-\theta_k)\,d\theta.$$

$$= (1+O(n^{-c}))\frac{2^{|E(G))|}}{\sqrt{t(G)}}\left(\frac{2}{\pi}\right)^{(n-1)/2}\mathbb{E}e^{f_M(X_t)},$$

$$f_M(\theta) := \sum_{\ell=2}^{M} c_{2\ell}\sum_{jk\in G}(\theta_j-\theta_k)^{2\ell}.$$

where $c_{2\ell}$ are the coefficients of expansion of $\log\cos x$ around $x=0$,

$$c_{2\ell} := \frac{(-4)^{\ell}(1-4^{\ell})B_{2\ell}}{2\ell(2\ell)!}.$$

We also employ *cumulant expansion*

$$\log\mathbb{E}e^{tW} = \sum_{r=1}^{\infty}\frac{t^r}{r!}\kappa_r(W).$$

Cumulant tail bound

Good news: $\kappa(f_M(X_t)) \sim \kappa_r(f_M(X))$ for any fixed r (or slowly growing).

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Motivation:

- Edgeworth expansion for U-statistics $\sum_{j<k} h(X_j, X_k)$.
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Motivation:

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We proved a new bound on the tail of cumulant expansion for f, provided $D_V(f)$ decreases sufficiently fast wrt to the size of $V \subseteq \{1, \ldots, n\}$.

$$D_V(f) := \sup_{x,y} |\partial_y^V [f](x)|,$$

where $\partial_y^V := \partial_y^{v_1} \cdots \partial_y^{v_k}$ and

$$\partial_y^j [f](x) := f(x) - f(x_1, \ldots, x_{j-1}, y_j, x_{j+1}, \ldots x_n).$$

New formula for Eulerian orientations

Theorem 3 (Isaev, McKay, Zhang, 2023)

Let $\Delta \gg \log^8 n$ and $h(G) \geqslant \gamma\Delta$ for some fixed $\gamma > 0$. Let $c > 0$ be a constant and $M := \left\lceil \frac{c \log n}{\log \Delta - 4 \log\log n} \right\rceil$. Then, as $n \to \infty$

$$\mathrm{EO}(G) = \frac{2^{|E(G)|}}{\sqrt{t(G)}} \left(\frac{2}{\pi}\right)^{\frac{n-1}{2}} \exp\left(\sum_{r=1}^{M} \frac{1}{r!}\,\kappa_r\left(f_M(X)\right) + O(n^{-c})\right),$$

where X is a singular Gaussian with density proportional to $e^{-\frac{1}{2}x^T L x}$.

Good precision for regular tournaments

Corollary

For odd $n \to \infty$, we have

$$\mathbf{EO}(K_n) = \left(\frac{n}{e}\right)^{1/2} \left(\frac{2^{n+1}}{\pi n}\right)^{(n-1)/2} \exp\Bigg(\frac{1}{4n} + \frac{1}{4n^2} + \frac{7}{24n^3} + \frac{37}{120n^4} + \frac{31}{60n^5} + \frac{81}{28n^6} + \frac{5981}{336n^7} + \frac{22937}{240n^8} + \frac{90031}{180n^9} + \frac{1825009}{660n^{10}} + \frac{4344847}{264n^{11}} + O(n^{-12})\Bigg).$$

For example, $\mathbf{EO}(K_{11}) = 48251508480$.

drop term	value	rel. err.	drop term	value	rel. err.
$O(n^{-1})$	4.7058280×10^{10}	2.5×10^{-2}	$O(n^{-7})$	4.8251420×10^{10}	1.8×10^{-6}
$O(n^{-2})$	4.8140033×10^{10}	2.3×10^{-3}	$O(n^{-8})$	4.8251464×10^{10}	9.2×10^{-7}
$O(n^{-3})$	4.8239598×10^{10}	2.5×10^{-4}	$O(n^{-9})$	4.8251486×10^{10}	4.7×10^{-7}
$O(n^{-4})$	4.8250171×10^{10}	2.8×10^{-5}	$O(n^{-10})$	4.8251496×10^{10}	2.6×10^{-7}
$O(n^{-5})$	4.8251187×10^{10}	6.7×10^{-6}	$O(n^{-11})$	4.8251501×10^{10}	1.5×10^{-7}
$O(n^{-6})$	4.8251341×10^{10}	3.5×10^{-6}	$O(n^{-12})$	4.8251504×10^{10}	9.3×10^{-8}

Residual entropy estimates

Pauling is right for random graphs!

The following quantity is important for ice-type models:

$$\rho(G) := \frac{1}{n} \log \mathrm{EO}(G).$$

Pauling's estimate gives

$$\mathrm{Pauling}(G) := \frac{1}{n} \sum_{j=1}^{n} \log \binom{d_j}{d_j/2} - \frac{\sum_{j=1}^{n} d_j}{2n} \log 2.$$

Theorem 4 (Isaev, McKay, Zhang)

If $\Delta^2 = o(n)$ or $\Delta/\delta = O(1)$ then

$$\Pr\Big(\rho(G) \sim \mathrm{Pauling}(G)\Big) \geqslant 1 - e^{-\Omega(n)},$$

where G is a random graph with degrees $d_1, \ldots, d_n$.

Correction to Pauling's estimate

For a d-regular graph G, we have

$$\mathrm{Pauling}(G) = \log \binom{d}{d/2} - \frac{d}{2} \log 2.$$

Under the assumptions of Theorem 3, we have

$$\rho(G) \approx -\frac{1}{2n} \log t(G) + \frac{d}{2} \log 2 - \frac{n}{2} \log \frac{\pi}{2} + \text{cumulants}.$$

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Idea: $\boxed{\rho(G) + \frac{1}{2n} \log t(G) \text{ depends less on the structure of } G.}$

We introduce the following correction to Pauling's estimate:

$$\hat{\rho}(G) := \mathrm{Pauling}(G) + \frac{1}{2}\tau_d - \frac{1}{2n} \log t(G)$$

where $\tau_d = \log \frac{(d-1)^{d-1}}{(d^2-2d)^{d/2-1}}$ is the typical value of $\frac{1}{n} \log t(G)$.

Square lattice L_n

Lieb's square ice constant is $\lim_{n\to\infty} \mathrm{EO}(L_n)^{1/n} = \frac{8\sqrt{3}}{9}$. Thus,

$$\rho(L_n) = \log\left(\frac{8\sqrt{3}}{9}\right) \approx 0.4315.$$

Pauling's estimate gives

$$\mathrm{Pauling}(L_n) = \log 1.5 \approx 0.4055.$$

From [Glasser, Wu, 2005] we know that

$$\frac{1}{n}\log t(L_n) = \frac{4}{\pi}\sum_{j\geq 1}\frac{\sin(j\pi/2)}{j^2}.$$

We also have $\tau_4 = \log\frac{27}{8}$. Then, our estimate gives

$$\hat{\rho}(G) = \mathrm{Pauling}(L_n) + \frac{1}{2}\tau_4 - \frac{2}{\pi}\sum_{j\geq 1}\frac{\sin(j\pi/2)}{j^2} \approx 0.4306.$$

Triangular lattice T_n

Baxter's constant is $\lim_{n\to\infty} \mathrm{EO}(T_n)^{1/n} = \frac{3\sqrt{3}}{2}$. Thus,

$$\rho(T_n) = \log\left(\frac{3\sqrt{3}}{2}\right) \approx 0.9548.$$

Pauling's estimate gives

$$\mathrm{Pauling}(T_n) = \log 2.5 \approx 0.9163.$$

From [Glasser, Wu, 2005] we know that

$$\frac{1}{n}\log t(T_n) = \frac{4}{\pi}\sum_{j\geq 1}\frac{\sin(j\pi/3)}{j^2}.$$

We also have $\tau_6 = \log \frac{5^5}{24^2}$. Then, our estimate gives

$$\hat{\rho}(T_n) = \mathrm{Pauling}(T_n) + \frac{1}{2}\tau_6 - \frac{2}{\pi}\sum_{j\geq 1}\frac{\sin(j\pi/3)}{j^2} \approx 0.9542.$$

3D cubic lattice C_n

The asymptotics is an open question. We computed

$$\rho(C_{125}) \in [0.94108, 094116], \qquad \rho(C_{216}) \in [0.9342, 0.9351].$$

Pauling's estimate gives

$$\mathbf{Pauling}(C_n) = \log 2.5 \approx 0.916.$$

From [Rosengren, 1987], we know that

$$\frac{1}{n} \log \tau(C_n) \approx 1.673.$$

We also have $\tau_6 = \log \frac{5^5}{24^2}$. Then, our estimate gives

$$\hat{\rho}(C_n) = \mathbf{Pauling}(C_n) + \frac{1}{2}\tau_6 - \frac{1.673}{2} \approx 0.925.$$

Hypercube Q_d on $n = 2^d$ vertices

We computed

$$\rho(Q_6) \approx 0.955, \qquad \rho(Q_8) \approx 1.489.$$

Pauling's estimate gives

$$\mathbf{Pauling}(Q_6) \approx 0.916, \qquad \mathbf{Pauling}(Q_8) \approx 1.476.$$

From [Bernardi, 2012], we know that

$$t(Q_d) = \frac{1}{n} \prod_{i=1}^{d} (2i)^{\binom{d}{i}}.$$

We also have $\tau_6 = \log \frac{5^5}{24^2}$, $\tau_8 = \log \frac{7^7}{48^3}$. Then, our estimate gives

$$\hat{\rho}(Q_6) \approx 0.948, \qquad \hat{\rho}(Q_8) \approx 1.489.$$

Thank you for listening!