Lattice enumeration

Nathan Clisby
The University of Melbourne

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Outline:

- Lattice models
- Critical phenomena
- Description of the finite lattice method
- Application to self-avoiding polygons
- Will focus on the "what" and the "how" of the finite lattice method, and leave the big picture to Tony and Ian.

Lattice models

- Lattice models are used to approximate physical systems, to gain understanding of collective behaviour known as phase transitions.
- Most famous such model is the Ising model, which assigns a magnetic spin variable to each site of the lattice.
- In order to understand properties of lattice models, need to calculate the partition function which is a sum over all possible configurations with appropriate (Boltzmann) weights.
- For the square lattice this was solved exactly by Onsager in 1942.

Lattice models

- When the system has a phase transition we expect that thermodynamic functions will have a singularity critical point.
- The corresponding critical exponent controls how the function behaves in the vicinity of the critical point. E.g.,

$$\chi(x) = A(x)\left(1 - \frac{x}{x_c}\right)^{-\gamma} + \text{corrections}$$
$$= \sum_{n=0}^{\infty} c_n x^n$$
$$\Rightarrow c_n \sim A^* n^{\gamma-1} x_c^{-n} = A^* n^{\gamma-1} \mu^n$$

- Exact solutions (for some 2d models) give us exact exponents; enumerations and Monte Carlo give us approximate but accurate exponents.

Lattice models

- What makes this exercise more than an interesting mathematical game is that we find that lattice models, like real physical systems, lie in distinct universality classes.
- Critical exponents are universal quantities, and so our simple, unphysical model has the same critical exponents as real physical systems.
- Loosely, at the critical point there are long range correlations, which are much longer than the short distance details of any particular model. Thus models with the same kinds of correlations are indistinguishable when we view them at a sufficiently large length scale.
- Formalised by the renormalisation group of Ken Wilson, for which he won the Nobel Prize in 1982.

Lattice enumeration

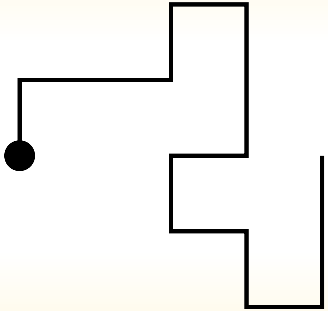
- For lattice models, it is possible to calculate the coefficients c_n via a graphical expansion.
- These calculations are *combinatorial*, and the partition function and related quantities can be written as infinite series with integer or rational coefficients.
- As early as the late 1940's Cyril Domb pioneered the use of series expansions to study lattice models, and he established a school at King's College London which developed this powerful approach and applied it to a wide range of problems.

Self-avoiding walks and polygons

- Self-avoiding walks are walks on a lattice that start at the origin and can never revist any site.
- Self-avoiding polygons return to the origin.

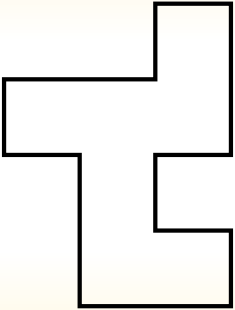
Self-avoiding walks and polygons

Self-avoiding walk of 15 steps on the square lattice



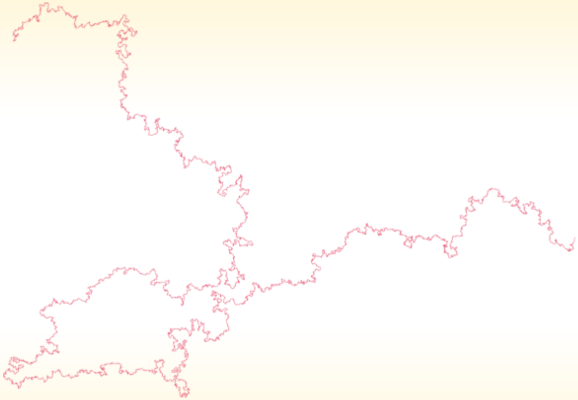
Self-avoiding walks and polygons

Self-avoiding polygon of 16 steps on the square lattice



Self-avoiding walks and polygons

Self-avoiding walk of 2^{25} steps on the square lattice



Self-avoiding walks and polygons

It is widely believed that the following asymptotic behaviour occurs for the self-avoiding walk in any dimension:

$$
\begin{aligned}
p_n &\sim B\mu^N n^{\alpha-2} \\
c_n &\sim A\mu^N N^{\gamma-1} \\
\langle R_{\mathrm{e}} \rangle_n &\sim D n^{2\nu}
\end{aligned}
$$

In 2d, $\alpha = 1/2$, $\gamma = 43/32$, $\nu = 3/4$.
In 3d, $\alpha \approx 0.23$, $\gamma = 1.156957(9)$, $\nu = 0.587597(7)$.

Self-avoiding walks and polygons

- Physically, self-avoiding walk correspond to the universality class of polymers (long-chain molecules) in a good solvent.
- ν, which determines how the size of the walk grows with the number of steps, can be measured experimentally for a range of so-called homopolymers.
- It has been found to correspond exactly with the value of ν for self-avoiding walks. In the context of polymers, ν is known as the Flory exponent.

Enumeration

- Brute force: μ^n, where $\mu \approx 2.63$.
- Guiding principle for efficient enumeration: if it's too hard, transform your problem and count something less numerous instead.
- Various games can be played for SAW, Sykes and others counted dumbbells and other configurations, more recently Clisby, Liang, and Slade[1] used the "lace expansion".
- This only gets you a polynomial factor.
- Finite lattice method (FLM) makes an exponential improvement.

[1] N. Clisby/R. Liang/G. Slade: Self-avoiding walk enumeration via the lace expansion, J. Phys. A: Math. Theor. 40 (2007).

The finite lattice method

- FLM was pioneered by Ian and Tom de Neef (1977, and a little earlier)[2], initially applied to the Potts model (a generalisation of the Ising model).
- Longer series, with sophisticated methods of series analysis (e.g. differential approximants) can allow dramatically better estimates of universal quantities.
- This combination formed the basis of the collaboration between Ian Enting and Tony Guttmann over the past 30+ years.
- Will go through a toy example to demonstrate the basic principle (hard squares on a small rectangle).
- Then move on to self-avoiding polygons.

[2] T. de Neef/I. G. Enting: Series expansions from the finite lattice method, J. Phys. A: Math. Gen. 10 (1977).

From Enting (1980)[3]: *"The finite lattice method involves three stages, two formal and one computational.*
(i) The series expansion has to be formally expressed as a linked-graph expansion.
(ii) Formally, the linked-graph expansion has to be re-expressed as a sum of contributions from finite rectangles.
(iii) The contributions for finite rectangles must be computed and then combined in the appropriate way."

[3] I. G. Enting: Generating functions for enumerating self-avoiding rings on the square lattice, J. Phys. A: Math. Gen. 13 (1980).

Enting (1980)[4], continued: *"Of these steps: (i) the linked-graph formulation was known for many models long before the finite lattice method was first described; (ii) the resummation is given once and for all by Enting (1978); (iii) the contributions from rectangles can be computed efficiently by using techniques based on a transfer matrix formalism.*

In the enumeration of polygons we are only concerned with connected graphs, and so the formal aspects of the combinatorics involve ensuring that the generating functions exclude all contributions from two or more co-existing polygons."

A brilliant combinatorial insight by Ian allowed him to specify the boundary so that only genuine polygons were counted, and the LHS and RHS were kept independent.

This key paper was one of Ian's first at CSIRO! "Present address: CSIRO, Atmospheric Phys., PO Box 77 Mordialloc Vic. 3195, Australia."

[4] Enting: Generating functions for enumerating self-avoiding rings on the square lattice (see n. 3).

Finite lattice method for SAPs

- Reduce the problem of enumerating all SAPs (of length $\leq N$) to that of enumerating all SAPs within minimum bounding rectangles:

$$P(x) = \sum_{W=1}^{\infty} P_{W\times W}(x) + 2\sum_{L=1}^{\infty}\sum_{W=1}^{L-1} P_{W\times L}(x).$$

- Define boundary states so that when a boundary between two parts of the rectangle is fixed, then the partial generating functions to the LHS and the RHS of the boundary are independent of each other.

$$P_{W\times L}(x) = \sum_{b_i\in\{\text{boundary states}\}} P^{(b_i)}_{W\times L,\text{LHS}}(x) P^{(b_i)}_{W\times L,\text{RHS}}(x)$$

Finite lattice method for SAPs

- These boundary states specify the topology of the SAP either to the left or the right of the boundary.
- For the square lattice, each edge can have 3 states.
- We have $2(W+L) \leq n$, and $W \leq L$, so $W \leq n/4$.
- Number of boundary states bounded by $3^{W+1} \sim 3^{n/4}$.
- Hence instead of generating $2.638\cdots^n$ SAPs, we generate $(3^{1/4})^n = (1.31\cdots)^n$ boundary states.
- Pruning allows you to do even better, roughly 1.20^n.

Results for self-avoiding polygons

- Sykes et al. (1972)[5] $p_{26} = 14\,385\,376$.
- Enting (1980)[6] $p_{38} = 636\,737\,003\,384$ (FLM).
- Guttmann and Enting (1988)[7] $p_{56} = 9\,293\,993\,428\,791\,901\,042$ (metric properties).
- Jensen and Guttmann (1999)[8] $p_{90} = 600\,931\,442\,757\,555\,468\,862\,970\,353\,941\,700$ (pruning).

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[5] M. F. Sykes/A. J. Guttmann/M. G. Watts/P. D. Robers: The asymptotic behaviour of selfavoiding walks and returns on a lattice, J. Phys. A: Math. Gen. 5 (1972).

[6] Enting: Generating functions for enumerating self-avoiding rings on the square lattice (see n. 3).

[7] A. J. Guttmann/I. G. Enting: The size and number of rings on the square lattice, J. Phys. A: Math. Gen. 21 (1988).

[8] I. Jensen/A. J. Guttmann: Self-avoiding polygons on the square lattice, J. Phys. A: Math. Gen. 32 (1999).

Results for self-avoiding polygons

- Jensen[9] $p_{110} =$
  97 148 177 367 657 853 074 723 038 687 712 338 567 772.
  (parallel implementation).
- Clisby and Jensen[10] $p_{130} =$
  17 076 613 429 289 025 223 970 687 974 244 417 384 681 143 572 320
  (constrain future topology)
- The extended series in[11] yielded:
  the estimates $x_c^2 = 0.143680629269(2)$,
  $\mu = 2.63815853035(2)$, $\alpha = 0.500000015(20)$.

[9] I. Jensen: A parallel algorithm for the enumeration of self-avoiding polygons on the square lattice, J. Phys. A: Math. Gen. 36 (2003).

[10] N. Clisby/I. Jensen: A new transfer-matrix algorithm for exact enumerations: self-avoiding polygons on the square lattice, J. Phys. A: Math. Theor. 45 (2012).

[11] Ibid.

What's next?

- FLM as a tool to explore boundary of solvable models - conjecturing exact results.
- Recent improvements will allow efficient FLM for 3d walk and polygon models, since pruning problem has been solved.
- Surprisingly, more than 30 years since FLM was first applied to SAWs and SAPs progress is still being made in improving the method.