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Upper bounds on the growth rates of independent sets in two dimensions via corner transfer matrices

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A B S T R A C T

We devise an algorithm to calculate upper bounds on the growth rates of the number of independent sets on a variety of regular two-dimensional lattices, using an amalgamation of techniques from linear algebra, combinatorics, and statistical mechanics. Our method uses Calkin and Wilf's transfer matrix eigenvalue upper bound together with the Collatz–Wielandt formula from linear algebra. To obtain a good bound, we need an approximate eigenvector, which we find using Baxter's corner transfer matrix ansatz and Nishino and Okunishi's corner transfer matrix renormalisation group method. This results in an algorithm for computing upper bounds which is far faster in practice than all other known methods. It is also the first algorithm for this problem with a polynomial, rather than exponential, memory requirement, and it is extremely parallelisable. This allows us to make dramatic improvements to the previous best known upper bounds. We apply our algorithm to five models, including independent sets on the square lattice (also known as the hard squares lattice gas from statistical mechanics). In all cases we extend the number of rigorously known digits of the growth rate by 4–6 digits.

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1. Introduction

We study the problem of independent sets on two-dimensional lattices. An independent set on a graph is defined to be a set of vertices of the graph such that no two vertices in the set are connected by an edge. We are interested in enumerating the number of such sets on a graph, known as the Merrifield–Simmons index [1,2]. More specifically, we wish to study the asymptotic growth of the number of independent sets on a regular lattice as the number of vertices in the graph grows to ∞.

Consider a regular lattice G with N spins. We wish to calculate the Merrifield–Simmons index

$$\sigma(G) = \#\text{ of independent sets on } G. \tag{1}$$

This quantity typically grows exponentially with respect to the number of vertices N; hence we seek to calculate the *growth rate* of this quantity, defined as

$$\kappa = \lim_{N\to\infty} \sigma(G)^{1/N}. \tag{2}$$

This problem is very closely related to magnetic spin models from statistical mechanics. In these models, magnetic spins are placed at the vertices of a regular lattice. In the simplest case, each spin can take one of two values, denoted ● and ○ (representing "up" or "down" spins, or alternatively "occupied" and "vacant" sites). In addition, there is also a constraint on the validity of spin configurations; disallowing configurations where two ● vertices are adjacent corresponds to the independent sets problem.

Taking the underlying lattice to be a square lattice results in the most famous model of this type, the hard squares lattice gas. This model can be considered to represent a gas of particles. A ● spin represents a particle, while a ○ spin represents a vacuum (absent particle). There is a close-range interaction between particles, which we represent by not allowing two particles to be nearest neighbours on the lattice. If we think of each ● spin as being the centre of a square plaquette (rotated by 45°), then this constraint forbids these plaquettes from overlapping, hence the name of the model.

In statistical mechanics, the quantity of interest is the *partition function*

$$Z_N = \sum_{\text{all valid configurations on } N \text{ spins}} z^{\#\text{ of } \bullet \text{ spins in the configuration}}, \tag{3}$$

where z is a fugacity variable which weights the ● spins. The partition function determines the physical properties of the model, such as free energy and phase transitions. It is clear that the $z = 1$ case corresponds directly to the number of independent sets on a square lattice.

These models also arise in simple models of constrained data storage on magnetic tape. As the tape is read from left to right, a ○ spin indicates that the current bit is equal to the previously read bit, while an ● spin indicates that it is the opposite. Due to