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On the Ising problem and some matrix operations

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Akademisk avhandling

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Abstract. The first part of the dissertation concerns the Ising problem proposed to Ernst Ising by his supervisor Wilhelm Lenz in the early 20s. The Ising model, or perhaps more correctly the Lenz-Ising model, tries to capture the behaviour of phase transitions, i.e. how local rules of engagement can produce large scale behaviour.

Two decades later Lars Onsager solved the Ising problem for the quadratic lattice without an outer field. Using his ideas solutions for other lattices in two dimensions have been constructed. We describe a method for calculating the Ising partition function for immense square grids, up to linear order 320 (i.e. 102400 vertices).

In three dimensions however only a few results are known. One of the most important unanswered questions is at which temperature the Ising model has its phase transition. In this dissertation it is shown that an upper bound for the critical coupling K_c, the inverse absolute temperature, is 0.29 for the tree dimensional cubic lattice.

To be able to get more information one has to use different statistical methods. We describe one sampling method that can use simple state generation like the Metropolis algorithm for large lattices. We also discuss how to reconstruct the entropy from the model, in order to obtain parameters as the free energy.

The Ising model gives a partition function associated with all finite graphs. In this dissertation we show that a number of interesting graph invariants can be calculated from the coefficients of the Ising partition function. We also give some interesting observations about the partition function in general and show that there are, for any N, N non-isomorphic graphs with the same Ising partition function.

The second part of the dissertation is about matrix operations. We consider the problem of multiplying them when the entries are elements in a finite semiring or in an additively finitely generated semiring. We describe a method that uses $\mathcal{O}\big(n^3/\log n\big)$ arithmetic operations.

We also consider the problem of reducing $n \times n$ matrices over a finite field of size q using $\mathcal{O}\big(n^2/\log_q n\big)$ row operations in the worst case.

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Introduction

I have mainly studied two problems, namely the Ising problem and matrix operations over finite fields. The focus in both cases has been on algorithms and in doing exact calculations on sometimes not so small examples since I like to see more than theoretic results. I am after all an applied mathematician.

The Ising problem

We observe a lot of phase transitions in the world around us, ice melts to water and water boils to vapour for example. The study of phase transitions is the study of how local rules can govern global behaviour. Under certain conditions small local changes can have a huge impact on the global behaviour. The most studied model for this is the Ising model.

To state the Ising partition function we need some definitions. Let $G = (V, E)$ be a graph with $n = |V|$ vertices and $m = |E|$ edges. Let $\sigma : V \to \{\pm 1\}$ be a function on the vertices, also known as *states*. Define the *energy* of the graph G as $\nu = \sum_{uv} \sigma(u)\sigma(v)$ and the *magnetization* as $\mu = \sum_{v} \sigma(v)$, where the sums are taken over all the edges $uv \in E$ and vertices $v \in V$ respectively. Now the *Ising partition function* is defined as

$$Z(G; x, y) = \sum_{\sigma} x^{\nu} y^{\mu}$$

where the sum is taken over all the 2^n states σ.

Furthermore we can define coefficients a_{ij} and a_i by the equations

$$Z(G; x, y) = \sum_{ij} a_{ij} x^i y^j \ , \ Z(G; x) = Z(G; x, 1) = \sum_{i} a_i x^i$$

It was not Ernst Ising but his thesis supervisor Wilhelm Lenz who first formulated the model known as the Ising model (in a paper from 1920 [Len20]). In this model the graph G is an infinite lattice in 1, 2, 3, ... dimensions. The formal variables x and y are evaluated in the temperature T as $x = \exp(-J/k_B T)$ and $y = \exp(-h/k_B T)$ respectively, where J is the interaction strength, h the outer field strength, k_B Boltzmann's constant ($1.3806505(24) \times 10^{-23}$ J / K) and T the temperature in Kelvin. What one now seeks is a singularity in the second derivative of $Z(G; \exp(-J/k_BT), \exp(-h/k_BT))$ as a function of T which is correlated to a phase transition. One of Lenz first Ph.D. students was Ising who was asked to study this model in late 1922. Ising did this and found the exact solution in one dimension (i.e. for paths and cycles). His result was published in a short paper in 1925 [Isi25].

The mathematical concept of the Ising-model seems to have been developed by the Cambridge group led by R. H. Fowler in the 1930's [Bru67]. Fowler discussed rotations of molecules in solids in a paper from 1935[Fow35]. In 1938 J. G. Kirkwood [Kir38] developed a systematic method for expanding the partition function in the inverse powers of the temperature. He based his method on the semi-invariant expansion by T. N. Thiele. The method of series expansion has been used since then to find approximations for the partition function of the Ising model.

In 1944 Lars Onsager published the exact solution to the Ising problem for the two dimensional square grid in zero magnetic field (e.g. $h = 0$ or equivalently $y = 1$) [Ons44]. The exact partition function and other properties for two-dimensional lattices have since been deduced by others from Onsager's work. The solution in a non-zero magnetic field and in higher dimensions is still unknown. For a history up to around 1965 see [Bru67] and for a more modern introduction see [Cip87].

Now let $S \subseteq V$ be a subset of the vertices. A *cut* is the subset of edges that have precisely one endpoint in S. The coefficients a_i count twice the number of cuts of size $(m-i)/2$. Each cut is counted twice since when adding over all states each cut will occur once when $S = \sigma^{-1}(+1)$ and a second time when $S = \sigma^{-1}(-1)$. The coefficients a_{ij} count the cuts with $(m-i)/2$ edges and $(n-j)/2$ vertices in one part.

If we let an even subgraph be a subgraph where all vertices have an even degree and b_i be the number of such subgraphs with i edges the partition function can be reformulated as

$$\sum_i a_i e^{iK} = 2\cosh^m K \sum_i b_i \tanh^i K. \tag{1}$$

This result is often attributed to van der Waerden.

The Ising problem in one variable can thus be reduced to the study of even degree subgraphs.

Paper I In this paper we find an upper bound on the critical coupling i.e. that $K_c \leq 0.29$ for the three dimensional cubic lattice. We also show how one can obtain an approximation from the different series expansions that exists for different types of lattices and compare these with sampled data.

Paper II In paper II we describe a method for calculating the exact partition function in one variable for square grids of finite size. Kaufman and Kasteleyn showed that the Ising partition function for the rectangular grid graph $C_s \times C_t$ can be expressed as a linear combination of four polynomials. These polynomials in turn are given by the Pfaffians of four matrices and can be calculated as the (formal) square roots of four determinants. The calculation of these determinants can be simplified since the eigenvalues of the matrices are zeros of Chebyshev polynomials. Simplifications as removing double roots are also used. Using this method we calculate the partition function exactly for grids up to linear size 320, i.e. 102400 vertices. We also do a short physicists type of analysis where we compare the behaviour of the finite lattices with asymptotics (exact and conjectured) from the literature.

Paper III In this short paper we describe the sampling method we used to get the sampled data in e.g. paper I. We also discuss how to reconstruct the entropy from the model, from witch i.e. the free energy can be obtained. We look into the problem of critical fluctuations and critical slowing down. All this makes it possible to use simple state generation like the Metropolis algorithm even though the lattice is large.

Paper IV In this paper we describe some of the combinatorial interpretations of the various coefficients. We show how to calculate a number of interesting combinatorial graph invariants form the Ising partition function. We also show that this is not enough to uniquely determine the graph. It is also shown that for every N there exists a set with N graphs that all have the same Ising partition function.

Matrix multiplication

Paper V Matrix multiplication is an important operation in today's society since much of what computers do is linear algebra of some kind. If one could multiply matrices faster one could often save resources e.g. time or space. We have considered the problem of multiplying matrices over finite semirings and additively finitely generated semirings. If the generating set is small enough, in comparison with the size of the matrices, one can save some arithmetic operations compared to the naïve method going from $\mathcal{O}(n^3)$ to $\mathcal{O}(n^3/\log n)$ arithmetic operations. This is important for example when doing arithmetic in the Boolean ring or computing over the integers modulo a small number.

Matrix reduction

Paper VI This article sprung from the question if there exits an infinite family of larger and larger invertible matrices such that a superlinear number of row operations are needed to reduce the matrices to the identity matrix. We show that it is possible to reduce $n \times n$ matrices over a finite field of size q using $\mathcal{O}(n^2/\log_q n)$ row operations in the worst case. We also show that almost surely we need $\mathcal{O}(n^2/\log_q n)$ row operations to reduce an infinite sequence of matrices $\{M_n\}_{n=1}^{\infty}$ where each M_n, an $n \times n$ matrix over a field of size q, is chosen uniformly at random.

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