Monte Carlo Simulations of the 3-State Potts Model in 2D

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The two-dimensional Ising model in zero-field was first solved exactly in 1944 by Lars Onsager.[4] It describes a square lattice with nearest neighbour interactions, where each lattice point has with it associated a number (which we will refer to as spin) which may either be +1 or -1 and was originally meant as a model for magnets. The Hamiltonian in zero-field is[1]

$$H = -J_1 \sum_{j=1}^{\mathcal{M}} \sum_{k=1}^{\mathcal{N}} \sigma_{j,k}\sigma_{j,k+1} - J_2 \sum_{j=1}^{\mathcal{M}} \sum_{k=1}^{\mathcal{N}} \sigma_{j,k}\sigma_{j+1,k}, \tag{1.1}$$

with $\mathcal{M}$ and $\mathcal{N}$ the extent of the lattice in the x- and y-directions respectively and J_1 and J_2 the interaction strength between neighbours in respectively the x- and y-directions. In the case where the interaction strength in both directions is the same the Hamiltonian becomes[3]

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j, \tag{1.2}$$

where the bracket denotes summation over nearest neighbours.[1] In the ferromagnetic ground state ($J > 0$) all spins on the lattice are aligned in one of two possible directions (the direction is chosen when the mirror symmetry in the lattice plane is spontaneously broken as the lattice cools). The Hamiltonian is subject to toroidal boundary conditions in both directions, meaning $\sigma_{1,k} = \sigma_{\mathcal{M}+1,k}$ and $\sigma_{j,1} = \sigma_{j,\mathcal{N}+1}$. We are interested in the thermodynamic properties of the Ising Model. To that end we define the partition function

$$Z = \sum_{\sigma=\pm 1} e^{-\beta H} \tag{1.3}$$

$$= \sum_{\sigma=\pm 1} \prod_{j=1}^{\mathcal{M}} \prod_{k=1}^{\mathcal{N}} e^{\beta J_1 \sigma_{j,k}\sigma_{j,k+1}} \prod_{j=1}^{\mathcal{M}} \prod_{k=1}^{\mathcal{N}} e^{\beta J_2 \sigma_{j,k}\sigma_{j+1,k}}, \tag{1.4}$$

[1] Note that naively applying this Hamiltonian to calculate the lattice energy overcounts the energy by a factor of 2 since each bond is counted twice.

with $\beta = 1/k_B T$ and the sum running over every possible orientation of the spins on the lattice. Solving this requires a non-trivial amount of effort and it is best to refer to either Onsager[4], who systemically added one-dimensional Ising models together to create a two dimensional lattice, or Kasteleyn as described in [1], whose approach considerably simplifies the derivation by reducing it to a combinatorial problem.

The derivation introduces a sign ambiguity in Z which takes some additional care to resolve, but we can avoid having to deal with this by considering the free energy F in the thermodynamic limit[2] instead of the partition function

$$\begin{aligned} F &= -\frac{1}{\beta} \lim_{\substack{\mathcal{N}\to\infty \\ \mathcal{M}\to\infty}} \frac{1}{\mathcal{M}\mathcal{N}} \log(Z_{\mathcal{M},\mathcal{N}}) \\ &= -\frac{1}{\beta}\left[\log(2) + \frac{1}{2}\frac{1}{(2\pi)^2}\int_0^{2\pi} \mathrm{d}\theta_1 \int_0^{2\pi} \mathrm{d}\theta_2 \log\Bigg(\cosh(2\beta J_1)\cosh(2\beta J_2) \right. \\ &\qquad \left. - \sinh(2\beta J_1)\cos(\theta_1) - \sinh(2\beta J_2)\cos(\theta_2)\Bigg)\right]. \end{aligned} \tag{1.5}$$

F is an analytic function of the temperature T, except at one value, which we will call the critical temperature T_c. At this temperature we can define the equality

$$|z_1| = \frac{1-|z_2|}{1+|z_2|}, \text{ with } z_1 = \tanh(2\beta J_1), z_2 = \tanh(2\beta J_2). \tag{1.6}$$

Rewritting and squaring this gives

$$1 - |z_1 z_2| = |z_1| + |z_2| \to \tag{1.7}$$
$$\left(1 - z_1^2\right)\left(1 - z_2^2\right) = 4\,|z_1 z_2| \tag{1.8}$$

Finally, using

$$\frac{1}{2z_k}\left(1 - z_k^2\right) = \frac{1}{\sinh(2\beta J_k)}, \text{ with } k \in \{1, 2\} \tag{1.9}$$

we get the equality

$$1 = \sinh(2\beta J_1)\sinh(2\beta J_2). \tag{1.10}$$

In the case where interaction strength in both the x- and y-directions is the same ($|J_1| = |J_2| = J$) we get an expression for the critical temperature in terms of the bond energy

$$1 = \sinh(2\beta J) \to \tag{1.11}$$
$$k_B T_c = \frac{2}{\operatorname{asinh}(1)} J = \frac{2}{\log\left(1+\sqrt{2}\right)} J \approx 2.269 J \tag{1.12}$$

[2]This is the limit in which the number of particles on the lattice tends to infinity.

Onsager [4] also calculated the values of the free energy, internal energy and entropy at the critical temperature[3]:

$$-\frac{f_c}{k_B T} = \frac{1}{2}\log 2 + \frac{2}{\pi} G \approx 0.929, \tag{1.13}$$

$$u_c = -\sqrt{2}J \approx -1.414J, \tag{1.14}$$

$$\frac{s_c}{k_B} = \log\left(\sqrt{2}e^{2G/\pi}\right) - \sqrt{2}\frac{J}{k_B T} \approx 0.306 \tag{1.15}$$

with G Catalan's constant.[4]

1.2.1 Thermodynamic Properties of the Two-Dimensional Ising Model

From the free energy it is relatively simple to determine the specific heat per spin and the internal energy per spin by taking the appropriate derivatives of the free energy[1]. We work with the isotropic case where $|J_1| = |J_2| = J$ and $z_1 = z_2 = z = \tanh(\beta J)$, corresponding to eq. (1.2). Then the expression for the free energy becomes

Check the formula in this part with [1], with special attention to factors of two and exponents!

$$\begin{aligned} F = -\frac{1}{\beta}\Bigg[&\log\Big(2\cosh^2(\beta J)\Big) + \log\Big(1+z^2\Big) \\ &+ \frac{1}{(2\pi)^2}\int_0^{\pi} \mathrm{d}\theta_1 \int_0^{\pi} \mathrm{d}\theta_2 \log\Big(1 - \frac{1}{2}k\Big\{\cos(\theta_1) + \cos(\theta_2)\Big\}\Big)\Bigg], \end{aligned} \tag{1.16}$$

with

$$k = \frac{4z(1-z^2)}{(1+z^2)^2} = \frac{2\sinh(2\beta J)}{\cosh^2(2\beta J)}. \tag{1.17}$$

Performing the substitutions $\omega_1 = \frac{1}{2}(\theta_1 + \theta_2)$ and $\omega_2 = \frac{1}{2}(\theta_1 - \theta_2)$ and integrating over ω_1 the free energy becomes

$$F = -\frac{1}{\beta}\left[\log(2\cosh(2\beta J)) + \frac{1}{\pi^2}\int_0^{\frac{\pi}{2}} \mathrm{d}\omega_1 \int_0^{\frac{\pi}{2}} \mathrm{d}\omega_2 \log\Big(1 - k\Big\{\cos(\omega_1) + \cos(\omega_2)\Big\}\Big)\right] \tag{1.18}$$

$$= -\frac{1}{\beta}\left[\log\Big(\sqrt{2}\cosh(2\beta J)\Big) + \frac{1}{\pi}\int_0^{\frac{\pi}{2}} \mathrm{d}\omega \log\Big(1 + \Big\{1 - k^2\cos^2(\omega)\Big\}^{\frac{1}{2}}\Big)\right] \tag{1.19}$$

We will take derivatives from this expression. The internal energy per spin is

$$u = \frac{\partial \beta F}{\partial \beta} \tag{1.20}$$

$$= -2J\tanh(2\beta J) + k\frac{\mathrm{d}k}{\mathrm{d}\beta}\frac{1}{\pi}\int_0^{\frac{\pi}{2}} \mathrm{d}\omega \frac{\sin^2(\omega)}{\Delta(1+\Delta)} \tag{1.21}$$

with

$$\Delta = \Big(1 - k^2\sin^2(\omega)\Big)^{\frac{1}{2}}. \tag{1.22}$$

[3] We use lowercase letters to denote the thermodynamic properties of a single spin on the lattice and uppercase letters when refering to the entire lattice. Taking as an example the internal energy, $U/N = u$ with N the number of spins on the lattice.

[4] $G = 1^{-2} - 3^{-2} + 5^{-2} - 7^{-2} \approx 0.916$

Note that the argument of the integral in eq. (1.20) can be rewritten as

$$\frac{\sin^2(\omega)}{\Delta(1+\Delta)} = \frac{(1-\Delta)\sin^2(\omega)}{\Delta(1-\Delta^2)} = \frac{1}{k^2}\left(\frac{1}{\Delta}-1\right), \tag{1.23}$$

from which it follows that

$$u = -2J\tanh(2\beta J) + \frac{1}{\pi}\frac{1}{k}\frac{\mathrm{d}k}{\mathrm{d}\beta}\left[K(k)-\frac{\pi}{2}\right]. \tag{1.24}$$

Here $K(k)$ is the complete elliptic integral of the first kind

$$K(k) = \int_0^{\frac{\pi}{2}} \frac{\mathrm{d}\phi}{\left(1-k^2\sin^2(\phi)\right)^{\frac{1}{2}}}. \tag{1.25}$$

Taking the derivative of k

$$\frac{1}{k}\frac{\mathrm{d}k}{\mathrm{d}\beta} = \frac{2J}{\tanh(2\beta J)}(1-2\tanh^2(2\beta J)), \tag{1.26}$$

the internal energy per spin becomes

$$u = \frac{-J}{\tanh(2\beta J)}\left[1+\frac{2}{\pi}\left\{2\tanh^2(2\beta J)-1\right\}K(k)\right]. \tag{1.27}$$

For the specific heat per spin we take the derivative of the internal energy per spin with respect to the temperature

$$c = \frac{\partial u}{\partial T} = \frac{-1}{k_B T^2}\frac{\partial u}{\partial \beta} \tag{1.28a}$$

$$\begin{aligned} &= \frac{J}{k_B T^2}\left[\frac{-2J}{\cosh^2(2\beta J)}\left\{1+\frac{2}{\pi}\left(2\tanh^2(2\beta J)-1\right)K(k)\right\}\right] \\ &\quad + \frac{16}{\pi}\frac{J}{\tanh^2 2\beta J}K(k) + \frac{2}{\pi}\frac{\left(2\tanh^2(2\beta J)-1\right)}{\tanh(2\beta J)}\frac{\mathrm{d}k}{\mathrm{d}\beta}\frac{\mathrm{d}K(k)}{\mathrm{d}k}. \end{aligned} \tag{1.28b}$$

For the derivative of the elliptic integral we use the identity[1]

$$\frac{\mathrm{d}K(k)}{\mathrm{d}k} = \frac{1}{kk'^2}\left[E(k)-k'^2K(k)\right], \tag{1.29}$$

where $E(k)$ is the complete elliptic integral of the second kind

$$E(k) = \int_0^{\frac{\pi}{2}} \mathrm{d}\phi \left(1-k^2\sin^2(\phi)\right)^{\frac{1}{2}}, \tag{1.30}$$

and $k'^2 = 1-k^2$. Using eq. (1.26) and eq. (1.30) the expression for the specific heat per spin becomes

$$c = k_B\left[\frac{\beta J}{\tanh(2\beta J)}\right]^2 \frac{2}{\pi}\left[2K(k)-2E(k)-\left(1-k'\right)\left\{\frac{\pi}{2}+k'K(k)\right\}\right]. \tag{1.31}$$

1.2.2 The Ising Model around T_c

Given that we would like to know how the Ising model behaves around T_c, we need to expand the expressions for the internal energy and the heat capacity around this temperature. When $T \approx T_c$ the argument k as defined in eq. (1.17) of the elliptic integrals in the definitions eq. (1.27) and eq. (1.31) becomes approximatly 1. More precisily

$$k \approx 1 - 4\beta_c^2 J^2 (\frac{T}{T_c} - 1)^2, \tag{1.32}$$

$$k^{'} \approx 2\sqrt{2}\beta_c J(\frac{T}{T_c} - 1) \tag{1.33}$$

with $\beta_c = \frac{1}{k_B T_c}$. It is obvious that for $k = 1$ $E(k) = 1$ whereas $K(1)$ diverges since the integral becomes

$$\int_0^{\frac{\pi}{2}} \frac{1}{\cos\theta} \, \mathrm{d}\theta \to \infty \tag{1.34}$$

Nevertheless an approximation around $k = 1$ yields $K(k) \approx \log\left(\frac{4}{k'}\right)$.

At T_c the internal energy per spin u does not diverge and has the value

$$u(T_c) = \frac{-J}{\tanh(2\beta_c J)} = -\sqrt{2}J. \tag{1.35}$$

The heat capacity per spin c does diverge. Using the previous expansions

$$\frac{c(T)}{k_B} \approx \frac{8}{\pi} (\beta_c J)^2 \left[\log\left(\frac{4}{k'}\right)\right] \tag{1.36}$$

$$= \frac{2}{\pi} \log\left(1 + \sqrt{2}\right)^2 \left[-\log\left(\frac{T}{T_c} - 1\right) - 1 - \frac{\pi}{4} - \log\left(\frac{\sqrt{2}}{4} \log\left(1 + \sqrt{2}\right)\right)\right] \tag{1.37}$$

and we see c diverging logarithmically as $T \to T_c$.

1.2.3 Magnetization of the Ising Model

1.3 The Potts Model

Chapter 2

Simulating Lattice Models

2.1 Markov Processes and Monte Carlo Methods

2.1.1 Ergodicity and Detailed Balance

2.2 The Metropolis Algorithm

The Metropolis algorithm, first published by Metropolis *et al.* in 1953 [2], is a simple algorithm that was first used by its creators to study the dynamics of continously displacable hard spheres.

2.2.1 Critical Slowing Down

2.3 The Wolff Algorithm

2.4 Generalizing Algorithms to the Potts Model

2.4.1 Optimizations

2.4.2 Systemic errors

Chapter 3

Analysis of Monte Carlo Simulations

Chapter 4

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5.1 Further Work

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