The 2-Dimensional Ising Model: Monte Carlo Simulation

Summary of Results from Other Approaches

• *The model:* The standard 2D Ising model consists of an $n \times n$ square lattice, at each site i of which is a spin $s_i = \pm 1$, with partition function (in the absence of an external field, with the usual definition $K := \beta J$)

$$Z(N,T) = \sum\nolimits_{\{s\}} \mathrm{e}^{K \, \Sigma'_{\langle ij \rangle} s_i s_j} \ .$$

• *Weiß mean-field theory:* This approximation gives a second-order phase transition in all dimensions D, at

$$T_{\mathrm{c}} = \frac{2DJ}{k_{\mathrm{B}}} \ , \qquad \text{or} \qquad K_{\mathrm{c}} = \frac{1}{2D} \ .$$

• *Analytic results:* An approximate treatment along the lines of Onsager's solution gives the result that there is spontaneous magnetization (corresponding to a second-order phase transition) below a critical temperature

$$T_{\mathrm{c}} = 2.269 \, J/k_{\mathrm{B}} \ , \quad \text{or} \quad K_{\mathrm{c}} = 0.44069 \ .$$

• *Renormalization group results:* Using an approximation to the larger theory with three coupling constants (K_1, K_2, K_3), one gets a simplified Kadanoff transformation $K' = \frac{3}{8} \ln \cosh(4K)$ which has, in addition to two stable fixed points at $K = 0$ and ∞, a non-trivial, unstable one at

$$K_{\mathrm{c}} = 0.50698 \ .$$

Monte Carlo Simulation – Setup

• *Setup:* Choose values for the system parameters:
– Lattice size (usually an $n \times n$ square, $n \mapsto$ `rows` in our Mathematica code),
– Coupling constant $K = \beta J$ (the "inverse temperature", called `Tinv` in our code), and
– Desired number `ncount` of configurations to be generated.
The value of `ncount` should be large enough that there is a high probability that the value of any quantity obtained by averaging over the generated spins is very close to the mean of that quantity over the canonical ensemble.

• *Initial configuration:* All initial configuration should lead to equivalent results, since the results will be considered reliable only after the simulation has had enough time to let the system "thermalize" anyway. One may choose a random-looking one or, for simplicity, one that is easy to set up. The ones that are currently implemented are:
– The "interface configuration" (the spins on the first `maxj` columns are $+1$, the remaining ones -1),
– The "checkerboard configuration" (the values of the spins alternate between $+1$ and -1), and
– The "random configuration" (each s_i is chosen independently at random, with probability p of being $+1$).
Whichever configuration is chosen, one needs to make sure that the desired boundary conditions are correctly implemented.

• *Procedure:* Applying the Metropolis algorithm, at each time step we
– Choose at random one lattice location,
– Tentatively change its spin value, $s_i \mapsto -s_i$, and
– Accept the change with probability $\min\{\mathrm{e}^{-K\Delta E}, 1\}$.

• *Thermalization:* Roughly speaking, a system has reached a typical configuration at temperature T when for each observable A the size of the oscillations around $\langle A \rangle$ coincides with the statistical uncertainty in $\langle A \rangle$. For this to happen, one must make sure that the system is ergodic and that a long enough time has passed. The best way to check this is to calculate correlations.

Monte Carlo Simulation – Simulation and Analysis

• *Analysis of magnetization:* If we want to determine the critical value $K_{\rm c}$, we can run the code with various values of K, keeping in mind the value we expect to find. After each simulation, a figure showing the value of the spin at each site, or a calculation of the spatial correlation function

$$\sigma_{ij} := \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \ ,$$

related to the susceptibility, will tell us more about long-range order than the value of $\langle s \rangle$ by itself does. The tricky part is to determine when the code has run long enough that the system can be considered to be thermalized, especially since near critical points systems approach equilibrium very slowly.

• *Response functions:* In a canonical ensemble, fluctuations of certain quantities are related to response functions. For example, for the magnetic susceptibility and the heat capacity,

$$\langle (\Delta M)^2 \rangle = k_{\rm B} T \, \chi \ , \qquad \langle (\Delta E)^2 \rangle = k_{\rm B} T^2 \, C_{\rm v} \ .$$

We can use this fact to help us determine whether a simulation has reached equilibrium by comparing the above value of $C_{\rm v}$ with the one from a more direct calculation,

$$C_{\rm v} = \frac{\langle E(T+\delta) - E(T-\delta) \rangle}{2\delta} \ .$$

• *Correlation decay time:* Another method we can use to find out how long it takes for a system to approximately reach equilibrium is to estimate the correlation decay time τ from the time dependence of the correlation. If the system is not near a critical point, we expect the correlation function for an observable x to be exponential in time,

$$\frac{\langle x(s+t)\, x(s) \rangle - \langle x \rangle^2}{\langle x^2 \rangle - \langle x \rangle^2} \approx {\rm e}^{-t/\tau} \ .$$

Reading

• *Pathria & Beale:* Mentioned in Sec 13.4; Problem 16.11.

• *Chandler:* Ch 5, pp 119 ff.
• *Halley:* pp 150–160.
• *Huang:* Chapter 12, especially Sec 12.9.
• *Mattis & Swendsen:* Secs 2.7–2.8, 8.5–8.10.
• *Plischke & Bergersen:* Chapter 9.
• *Reif:* Mentioned in p 429.
• *Schwabl:* Secs 6.5 and 7.3.