Simulating Glauber dynamics for the Ising model

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Why is it that many materials exhibit “spontaneous magnetization”?

- At low temperatures, they are magnetic.
- At high temperatures, they are not.

*Figure 8.* Magnetization-temperature curve of the powder calcined at 1450 °C when subsequently subjected to a 240 Oe magnetic field.
Electron “spins” and magnetization

• W. Lenz (1920) proposed a model of ferromagnetism. That each electron possesses a “spin”. Parallel spins attract. Antiparallel spins repel. At sufficiently low temperatures, the spins should align.

• Ernst Ising (1924), in his doctoral thesis advised by Lenz, formalized these ideas and examined a 1-D chain of such spins.

\[ s_i \in \{-1, +1\} \]

\[ E_i \propto -s_is_j \]

the “exchange energy”
The “Ising” model

- Consider a 2-D lattice.
- At each site is a spin, $s_i \in \{-1, +1\}$.
- Spins interact only with nearest neighbors.
- There can be an external field $h$.
- Thus the energy for each spin, $E_i$:

$$E_i = - \sum_{\{s_j\}} J_{ij} s_i s_j - h s_i$$
Total energy, the “Hamiltonian”

\[ \mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} s_is_j - \sum_i h s_i \]

- The first sum is over all nearest neighbor pairs.
- \( J_{ij} \) is the coupling between spins. We take \( J_{ij} = J = 1 \).
- Set external field \( h = 0 \) (if not, hysteresis).
  - Hysteresis enables magnetic storage of data.
  - Avalanche phenomena in domain flipping.
  - Studied via Random Field Ising Models (RFIM).
Magnetization, $M$

\[ M = \frac{1}{N} \sum_i s_i \]

- All spins “up” → $M = 1$.
- All spins “down” → $M = -1$.
Phase transition in $M$ as function of $T$

- Peierls (1936), gave a non-rigorous proof that spontaneous magnetization must exist for the 2-D Ising model.

- Onsager (1944), gave a complete analytic solution.

Phase transitions and universality — more on this later!
How to simulate the Ising model?

• Starting from any initial condition, we know the equilibrium value of the magnetization. It is a function only of Temperature. How do we get to equilibrium?
Equilibrium

- In equilibrium, Boltzmann probability:

\[ p(E_i) = \frac{e^{-E_i/kT}}{z} \]

- \( E_i \) is energy of state \( i \).
- \( k \) is Boltzmann’s constant.
- \( T \) is temperature.
- \( z = \sum_i e^{-E_i/kT} \) is the partition (i.e., generating) function.
Spin-flip algorithms
“Monte Carlo”

- Use a stream of random numbers to drive a stochastic process, in this case the generation of a succession of many states of the spin model.

- For an $L \times L$ lattice, there are $2^{L \times L}$ states. (e.g., If $L = 10$, there are $2^{100}$ possible states).

- Want to sample the phase space so that each state occurs with the same probability as its equilibrium probability.

- Metropolis (1953) detailed balance ensures convergence to equilibrium.

$$P(S_i)P(S_i \to S_j) = P(S_j)P(S_j \to S_i)$$
Detailed balance

\[ P(S_i)P(S_i \rightarrow S_j) = P(S_j)P(S_j \rightarrow S_i) \]

in other words:

\[ \frac{P(S_i \rightarrow S_j)}{P(S_j \rightarrow S_i)} = \frac{P(S_j)}{P(S_i)} = e^{-(E_j - E_i)/kT} \]

(Where the last equality follows from the Boltzmann probability).
Glauber dynamics

- $P(S_i \rightarrow S_j) = e^{-E_j/kT} / (e^{-E_j/kT} + e^{-E_i/kT})$
  
  $$= 1 / (1 + e^{\Delta E_{ji}/kT})$$

- Choose a spin at random.

- Calculate the energy difference resulting if that spin were flipped: $\Delta E$.

- Transition probability: $P(\text{flip}) = 1 / (1 + e^{\Delta E/kT})$.

- Generate a random number, $X$. If $X < P(\text{flip})$ accept.

- Parameterize time such that one unit of time is $N$ spin-flip attempts.
Implementing the Glauber dynamics

- Only a finite number (5) of possible energy changes.
- Can pre-compute the probabilities, $\frac{1}{1 + e^{\Delta E/kT}}$. 

\[ \begin{align*}
\text{Delta E} &= +/- 8 \\
\text{Delta E} &= +/- 4 \\
\text{Delta E} &= +/- 0 \\
\text{Delta E} &= -/+ 4 \\
\text{Delta E} &= -/+ 8
\end{align*} \]
Simulations

- High temperature (initial condition irrelevant)
- Low temperature (initial condition “quenched”)
- Critical temperature (???)
Issues

- Critical slowing down (correlation length diverges), and so does the relaxation time....

- The critical point is the most interesting, yet the hardest to access and pin down!
A coupled dynamics

- "Top" copy all spin up, +1.
- "Bottom" copy all spin down, -1.
Greedy coupled dynamics

- Pick a lattice site, $v$, at random.
- Calculate probability for spin $s_v$ to be $+1$ in the top, $p_{top}$.
- Calculate probability for spin $s_v$ to be $+1$ in the bottom, $p_{bot}$. 
Probabilities (as usual)

\[ p(+) = \frac{e^{-E(+)\beta}}{e^{-E(+)\beta} + e^{-E(-)\beta}} \]
Dynamics

- Generate a random number, $X$.
- Set $s_v$ to be blue if: $X < p_{bot}$.
- Set $s_v$ to be green if: $p_{bot} < X < p_{top}$.
- Set $s_v$ to be yellow if: $X > p_{top}$.
The coupled system

Growth of coupling with time.
Online Resources

Ising model simulation:

- http://stp.clarku.edu/simulations/ising2d/
- http://bartok.ucsc.edu/peter/java/ising/keep/ising.html

Cluster-flip dynamics: