Monte Carlo Modeling of Magnetic Phase Transitions

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Outline

- Background
- Introduction to the Model
- Monte Carlo Overview
- Preliminary Results
- Implementation and Observations
Background

- Individual atoms behave as miniature bar magnets
  - Atoms have a “spin” orientation
  - May interact with neighboring atoms

- Large-scale properties determined by tension between:
  - **Energy**: System prefers to be in a low-energy state (spins parallel)
  - **Entropy**: System prefers to be in a disordered state (spins random)

- Which prevails depends on temperature
- Phase transitions can occur between states
The Ising Model

- Assume atoms are arranged on a finite rectangular grid
- Atoms have two possible spins: up (+1) or down (−1)
- Energy of the system given by

\[
E = -J \sum_{\langle i,j \rangle} s_i s_j
\]

- From statistical physics, probability of any particular state:

\[
p = Z^{-1} e^{-\frac{E}{kT}}
\]
A First Attempt...

- Given a temperature $T$, what is the expected energy, $\langle E \rangle$?

- Answer: Compute weighted average over all possible configurations

- But... given $n$ atoms, there are $2^n$ configurations!

- We need a better method
Monte Carlo Methods

- Example: Compute $\pi$ by throwing darts
- Better than many other methods for large degree-of-freedom systems
- Error is approximately $1/\sqrt{\text{number of samples}}$
- Application to Ising Model:
  - Generate configurations at random
  - Compute summary statistic (such as energy) for each configuration
  - Average the results to get approximation for true value
- How to generate configurations which are representative?
Metropolis et al.

- Take a random walk in the configuration space
  - Only make small changes at each step
- In the Ising Model: choose a random atom to flip
- What would be the change in energy ($\Delta E$)?
  - If $\Delta E \leq 0$, flip the atom’s spin
  - If $\Delta E > 0$, flip with a probability of $e^{-\Delta E / kT}$
- Repeat... and repeat... and repeat...
- Surprisingly, gives the correct distribution
Some Results

- 160 × 160 square grid

\[ T = 1.20 \]
\[ T = 2.24 \]
\[ T = 4.00 \]
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Validation

- Observed the expected phase transition
  - Indicated by divergence of specific heat
- From literature, expected to observe at about $T_c = 2.236$
Implementation Details

- Actual implementation:
  - Lattice is $160 \times 160$, wraps at boundary
  - Start with $T = 0$, all spins parallel
  - Iterate about $20 \times \text{(number of atoms)}$ times
  - Print results
  - Increase $T$ by 0.02, repeat
  - $T$ increases to 4.00, falls to 0.00, and repeats once more
Difficulties

- How many iterations are needed to reach equilibrium?
- Some instances of non-equilibrium states observed:

\[ T = 1.20 \]
Future Work

- Only two-dimensional system considered thus far
- Expect to study other configurations
- Make more robust: iterate longer when necessary