Statistical Mechanics, Markov Chains and the Ising Model

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Statistical Mechanics:

Probability $\rho(\mathbf{S})$ to be in state S.

Ising model: $\mathbf{S} = \{S_i\}$,

Sites i on a (square) lattice $i = (x, y)$,

Spins $S_i = \pm 1$.

Equilibrium statistical mechanics:

Energy $E(\mathbf{S})$,

Boltzmann probability distribution

$\rho(\mathbf{S}) \propto \exp(-E(\mathbf{S})/k_B T)$.

High temperatures:

States have equal weight

Low temperaturatures:

Low-energy states predominate

Ising model: $E(\mathbf{S}) = -\sum_{\langle i,j \rangle} J S_i S_j$,

Lowest energy state ($J > 0$), all spins up (+1) or down (-1)

Broken symmetry ferromagnetic phase

High temperature, *paramagentic* phase

Transition at T_c: fluctuations

Markov chain:

Dynamics for statistical models

Transition rate $P_{\mathbf{S}'\mathbf{S}}$ from S to S′

Markovian: independent of history

Markov chain properties:

Detailed Balance:

Equilibrium flux $\mathbf{S} \to \mathbf{S}'$ = flux $\mathbf{S}' \to \mathbf{S}$

$P_{\mathbf{S}'\mathbf{S}} \cdot \rho(\mathbf{S}) = P_{\mathbf{S}\mathbf{S}'} \cdot \rho(\mathbf{S}') =$

Ergodic: Every state can be reached

A Markovian model that is ergodic and satisfies detailed balance will eventually approach equilibrium.

Ising model dynamics:

Heat bath:

Pick a spin at random, measure flip ΔE

Equilibrate it to it's current environment

Metropolis

Pick a spin at random, measure flip ΔE

If $\Delta E < 0$, flip down

If $\Delta E > 0$, some chance to flip up

Wolff algorithm

Clever generation of cluster flips

Vastly faster dynamics near T_c

Satisfies detailed balance, plus magic

Continuous-time; Bortz/Kalos/Lebowitz

- Keep lists of spins in different environments
- Calculate total rate to flip
- Find which spin environment flips next
- Flip random spin in that environment
- Vastly faster at cold temperatures
- Preserves dynamics (coarsening)