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Universität Bonn

Ising Model

A Statistical System at Finite Temperature

Simon Schlepphorst, Federico Diaz Capriles

Uni Bonn

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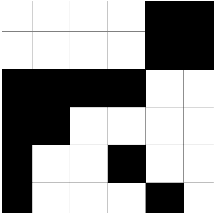
Introduction

Theory



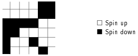
□ Spin up
■ Spin down

$$\mathcal{H}(\mathbf{s}) = -J \sum_{\langle i,j \rangle} s_i s_j \tag{1}$$

$$s_n \in \{-1, +1\}$$

$$\mathbf{s} = (s_1, s_2, \dots, s_N) \tag{2}$$

$$\mathcal{Z} = \sum_{\mathbf{s}} exp(-\frac{1}{k_B T}\mathcal{H}(s)) \tag{3}$$



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1. Describe graphic
2. Hamiltonian of the system. This is the $\mathcal{H}$ with no external field.
   J in this case denotes which type of interaction we have in our lattice:
   $J > 0 \rightarrow$ Ferromagnetic $\rightarrow$ Spins want to be alligned
   $J < 0 \rightarrow$ Antiferromagnetic $\rightarrow$ Spins want opposite of neighbors
   $J = 0 \rightarrow$ Noninteracting

3. Canonical Partition function. It would take a lot of time to go into detail on the Partition function (PF); but in a nutshell, it describes the statistical properties of the system and it represents a particular statistical ensemble.

Ising model can be difficult to evaluate numerically if there are many states for the system. For example, let:

L: Total number of sites in the lattice (length $\times$ width)
s_j: Spin state of the j-th point ($s_n \in \{-1, +1\}$)

With 2 states per spin, we have a total of 2^L possible configurations.
$\hookrightarrow$ Want to use Monte Carlo Methods

What can we find with MC? Estimates on the properties of the lattice

What does MC do? Use random number generation and accept reject methods to simulate lattice interaction

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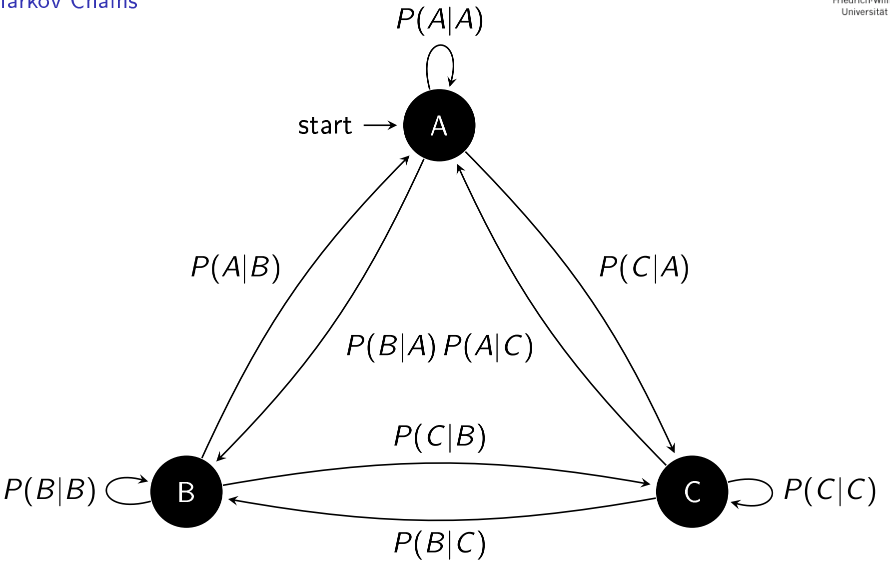
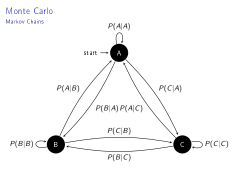
Some properties that can be estimated are: Specific heat or magnetization (at a given temperature)



$P(A|A)$
start
A
$P(A|B)$
$P(C|A)$
$P(B|A)$
$P(A|C)$
$P(C|B)$
$P(B|B)$
B
C
$P(C|C)$
$P(B|C)$



Markov Chains are mathematical systems that hop from one "state" (a situation or set of values) to another. That is to say, Markov chains tell you the probability to transition between states in a system.
So what takes us from state A to (lets say) state C is a series of jumps relying on probability.

We can build a transition matrix, P, which will then be used to describe the probability for any initial state, μ, to go to a final state, ν.

$$P = \begin{bmatrix} P_{11} & P_{12} & P_{13} & \dots & P_{1m} \\ P_{21} & P_{22} & P_{23} & \dots & P_{2m} \\ \vdots & \vdots & \vdots & P_{\mu\nu} & \vdots \\ P_{n1} & P_{n2} & P_{n3} & \dots & P_{nm} \end{bmatrix}$$

For physical systems, we require P to be irreducible and positive recurrent to ensure we "produce" the desired invariant distribution π_μ. This stationary distribution has the following properties:

$$\pi = \pi P \tag{4}$$

$$\pi_\mu P_{\mu\nu} = \pi_\nu P_{\nu\mu} \tag{5}$$

Where are our distributions?
Thermodynamical system $\rightarrow$ Boltzmann Statistics

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As we can see, we only have $\mu \rightarrow \nu$ transitions. That means that Markov chains are "memoryless" or that going to a state only relies on the state you are currently on and not any other step before that.

4. pi is a row vector in this notation.
5. definition of detailed balance

Irreducibility: Every state can be reached from any other state in a final numbe of steps.

Positive Recurrent: The chain returns to μ from μ in a finite time

Since we know our selection probabilities, $P_{\mu\nu}$ and π, we can now move on to making an accept-reject algorithm.
If we are on state X_n and want to test if we will transition to Y, we will do so with the following accept probability

$$X_{n+1} = \begin{cases} Y & \rho(X_n, Y_n) \\ X_n & 1 - \rho(X_n, Y_n) \end{cases} \tag{6}$$

$$\rho(X_n, Y_n) = min\left\{\frac{\pi_Y}{\pi_X}\frac{P_Y}{P_X}, 1\right\} = \frac{\pi_Y}{\pi_X}\frac{P_Y}{P_X} = \frac{\frac{1}{Z}e^{-\frac{\mathcal{H}_Y}{k_B T}}}{\frac{1}{Z}e^{-\frac{\mathcal{H}_X}{k_B T}}} = e^{-\frac{\mathcal{H}_Y - \mathcal{H}_X}{k_B T}} \tag{7}$$

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7. shows our acceptance/flip probability.
all thats left is just to apply all this in an algorithm.

1. Generate a lattice (hot, cold or random)
2. Pick a point
3. Test energy
4. If flipping benefits the lattice, then flip
5. Otherwise test against ρ with RGN
6. Repeat

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