

Ising Model

A Statistical System at Finite Temperature

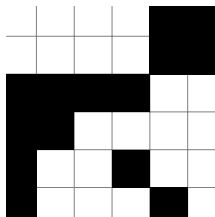
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1 Introduction

- Theory
- Monte Carlo Motivation
- Markov Chains
- Metropolis Algorithm



□ Spin up
■ Spin down

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

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

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

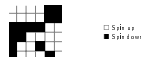
$$\mathcal{Z} = \sum_{\mathbf{s}} \exp\left(-\frac{1}{k_B T} \mathcal{H}(\mathbf{s})\right) \quad (3)$$

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

[1]

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

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

[2]

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

[3]

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 aligned
 $J < 0 \rightarrow$ 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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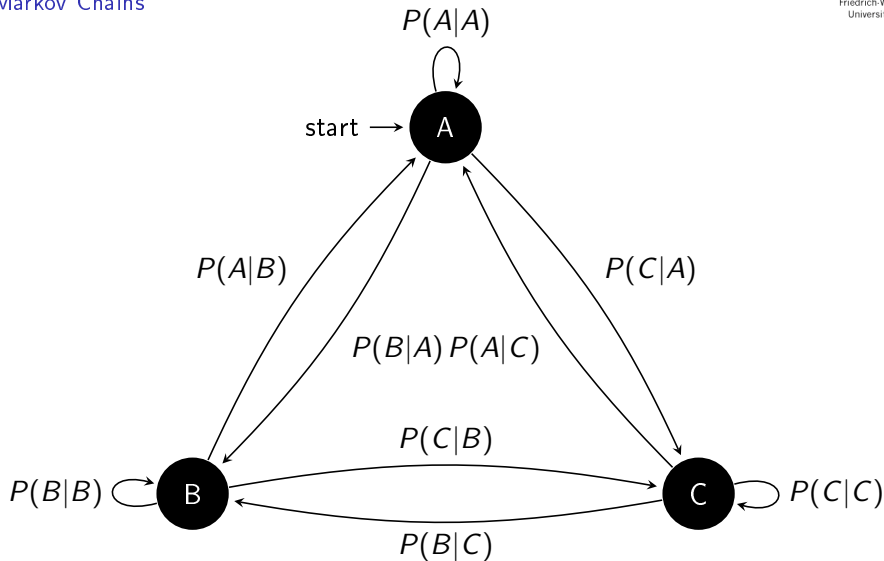
With 2 states per spin, we have a total of 2^L possible configurations.

→ We start to use Monte Carlo Methods

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

What does MC do? Use random sampling generation and accept/reject methods to simulate lattice behavior

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



2017-03-14

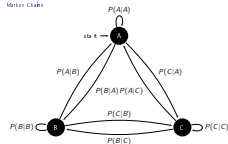
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Markov Chains



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

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

In the figure you can see a simple Markov Chain of 3 states. Furthermore, it is worth noting that $\sum_{s'} P(s'|s) = 1$
 We have a probability $P(y|x) \equiv P(x \rightarrow y)$

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We can build a matrix P which will be a stochastic matrix which will then be used to describe the probability for a system to go to a final state, y

$$\begin{bmatrix} P_{11} & P_{12} & P_{13} & \dots & P_{1n} \\ P_{21} & P_{22} & P_{23} & \dots & P_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ P_{n1} & P_{n2} & P_{n3} & \dots & P_{nn} \end{bmatrix}$$

In the figure you can see a simple Markov Chain of 3 states. Furthermore, it is worth noting that $\sum_x P(x \rightarrow y) = 1$.
We have a probability $P(y|x) = P(x \rightarrow y)$

We have prob for state x to go to y

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Metropolis Algorithm



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