

Markov-Chain Monte Carlo

Note Title

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Ising Model

$$\Lambda = \{-N, -N+1, \dots, N-1, N\}$$

$$\Omega = \{-1, 1\}^\Lambda = \{(\omega_{-N}, \omega_{-N+1}, \dots, \omega_{N-1}, \omega_N) : \omega_n \in \{-1, 1\}\}$$

For $\omega \in \Omega$, define

$$H(\omega) = \frac{1}{2} \sum_{j=-N}^{N-1} |\omega_{j+1} - \omega_j|^2$$



H is low if neighbors agree, large if a lot of "disorder"

$$L \subset \{-1, 1\}, \quad R \subset \{-1, 1\}$$

$$\Omega^{L,R} = \{\omega \in \Omega_N : \omega(-N) \in L, \omega(N) \in R\}$$



$$\tilde{P}_T^{L,R}(A) \stackrel{\text{def}}{=} \sum_{A \in \mathcal{B}(\Omega)} \dots$$

$$\frac{\sum_{\omega \in \Omega_N^{L,R}} \exp\left[-\frac{1}{T} H(\omega)\right]}{\sum_{\omega \in \Omega_N^{L,R}} \exp\left[-\frac{1}{T} H(\omega)\right]}$$

temperature

Partition function

$$Q: \tilde{E}^{a,b,T}(\omega(\omega)) = ?$$

How large is string of 1's around 0?

} large N

Need to Simulate

Idea: Find a Markov chain X with state space $\mathcal{R}^{a,b}$ having invariant measure μ . Then

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{j=1}^n f(X_j) = \tilde{E}_T^{L,R} [f]$$

Background: Detailed Balance & Reversibility

Definition: P a stochastic matrix, π a distribution. If

$$\pi_i P_{ij} = \pi_j P_{ji} \quad \text{all } i \neq j,$$

then π & P are in detailed balance

If so, then

$$\sum_i \pi_i P_{ij} = \sum_i \pi_j P_{ji} = \pi_j$$

So π is invariant. If P is irreducible & recurrent π is the only stationary distribution.

As long as $|I| < \infty$, irreducibility \Rightarrow recurrence.

Goal: Find P such that $P \neq \pi$ are in detailed balance. Use fact that Λ consists of "neighboring" sites

For $m \in \Lambda$, $\omega \sim \omega'$ if

$\exists n \in \Lambda$

$\omega(n) = \omega'(n)$ for all $n \neq m$.

Example for Ising Model ($L = R = \{-1, 1\}$)

$$\pi(\omega) \stackrel{\text{def}}{=} \frac{\exp\left(-\frac{1}{T} H(\omega)\right)}{\sum_{\omega' \in \Omega} \exp\left(-\frac{1}{T} H(\omega')\right)}$$

Start at $\omega \in \mathcal{R}$

(1) Pick an m (equal probabilities: $\frac{1}{2\pi\hbar}$)

(2) Change ω_m to $-\omega_m$ with

$$\omega' = (\omega_{-N} \dots -\omega_m \dots \omega_N)$$

probability

$$\frac{\pi(\omega) \sim \pi(\omega')}{\pi(\omega)} = \frac{\exp\left[-\frac{1}{T} H(\omega)\right] \sim \exp\left[-\frac{1}{T} H(\omega')\right]}{\exp\left[-\frac{1}{T} H(\omega)\right]}$$

don't need partition function

$$1 \sim \frac{\pi(\omega')}{\pi(\omega)} = 1 \sim \exp\left[-\frac{1}{T} \{H(\omega') - H(\omega)\}\right]$$

$$= 1 \sim \exp\left[-\frac{1}{2T} \left\{ |\omega_{m+1} + \omega_m|^2 + |\omega_{m-1} + \omega_m|^2 - |\omega_{m+1} - \omega_m|^2 - |\omega_{m-1} - \omega_m|^2 \right\}\right]$$

In other words, simulate a uniform (0,1) random variable U . If

$$U \leq \exp \left[-\frac{1}{2T} \left\{ |\omega_{m+1} + \omega_m|^2 + |\omega_{m-1} + \omega_m|^2 - |\omega_{m+1} - \omega_m|^2 - |\omega_{m-1} - \omega_m|^2 \right\} \right]$$

occurs with probability

$$1 \wedge \exp \left[-\frac{1}{2T} \left\{ |\omega_{m+1} + \omega_m|^2 + |\omega_{m-1} + \omega_m|^2 - |\omega_{m+1} - \omega_m|^2 - |\omega_{m-1} - \omega_m|^2 \right\} \right]$$

Then flip the m th site.

Then if $\omega \rightsquigarrow \omega'$ for some m ,

$$P_{\omega, \omega'} = \frac{1}{2N+1} \left\{ 1 \wedge \frac{\pi(\omega')}{\pi(\omega)} \right\}$$

↳ probability of flipping at site m

Detailed balance:

- If $\omega \stackrel{m}{\sim} \omega'$ for some m ,

$$\pi_{\omega} P_{\omega\omega'} = \frac{1}{2^{N+1}} \pi(\omega) \wedge \pi(\omega')$$

$$\pi_{\omega'} P_{\omega'\omega} = \frac{1}{2^{N+1}} \pi(\omega) \wedge \pi(\omega')$$

- If $\omega \not\stackrel{m}{\sim} \omega'$ for all m ,

$$\pi_{\omega} P_{\omega\omega'} = 0 = \pi_{\omega'} P_{\omega'\omega}$$

One can see that this system is irreducible.

Note: Could end up flipping at same site for several times. Could avoid this by sequencing through sites in a deterministic way.

Generalization Assume that ω_n could take on values $\{-L, -L+1, \dots, L\}$. Then we have more than one way to change the value at site n .

Note that above calculation came from requirement that

$$\pi_{\omega} P_{\omega\omega'} = \pi_{\omega} \wedge \pi_{\omega'}$$

Then

$$\pi_{\omega} P_{\omega\omega'} = \pi_{\omega'} P_{\omega'\omega}$$

should be symmetric
in $\omega \leftrightarrow \omega'$.

When $L \geq 1$, we should have a way of picking

How we want to change the n th site.

Start at $w \in \Omega$

(1) Randomly pick site m (equal probabilities)

$$p = \frac{1}{2N+1}$$

(2) Randomly pick (equal probabilities)

$$w \in \{-L, \dots, L\} \setminus \{w_m\}$$

$$\tilde{w} = \begin{cases} w_m & \text{if } u \neq m \\ w & \text{if } u = m \end{cases}$$

Metropolis
Algorithm

Generate U uniform $(0,1)$. Make the
transition to \tilde{w} if $U < 1 \wedge \frac{\pi_{\tilde{w}}}{\pi_w}$.

$$P_{w\tilde{w}} = \frac{1}{2N+1} \frac{1}{2L} \left\{ 1 \wedge \frac{\pi_{\tilde{w}}}{\pi_w} \right\} \quad \text{if}$$

site *way to flip* *acceptance prob.*

$$P_{w\tilde{w}} = 0 \quad \text{if } w \neq \tilde{w} \text{ for all } m$$

$$P_{ww} = 1 - \sum_{\substack{m \\ w \neq w'}} P_{ww}$$

If $\omega \sim \tilde{\omega}$,

$$\pi_{\omega} P_{\omega \tilde{\omega}} = \frac{1}{2^{N+1}} \frac{1}{2L} \{ \pi_{\omega} \pi_{\tilde{\omega}} \}$$

Another way

- ① Randomly pick site m (equal probabilities)
- ② Pick a way to flip with coordinates with likelihoods

$$P\{\omega^i\} = \frac{\pi_{\omega^i}}{\sum_{\omega'' \sim \omega} \pi_{\omega''}}$$

$C_m(\omega)$

Gibbs sampler

$$P_{w\tilde{w}} = \frac{1}{2N+1} \frac{\pi\tilde{\omega}}{C_n(\omega)}$$

\sim site
 \sim way to flip

$$P_{w\tilde{w}} = 0 \quad \text{if } w \neq \tilde{w} \text{ for all } m$$

$$P_{w\omega} = 1 - \sum_{\substack{m \\ w \neq \tilde{w}}} P_{w\omega}$$

$$\pi_{\omega} P_{w\tilde{w}} = \frac{1}{2N+1} \frac{\pi_{\omega} \pi_{\tilde{\omega}}}{C_n(\omega)} = C_n(\tilde{\omega})$$