Markov Chain Monte Carlo

Note Title 11/15/2006

Ising Model

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

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

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"

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

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

$$\tilde{\mathbb{P}}^{L,R}_{T}(A) \overset{\text{def}}{=} \frac{\sum_{\omega \in A \cap \Omega_N^{L,R}} \exp\left[-\frac{1}{T} H(\omega)\right]}{\sum_{\omega \in \Omega_N^{L,R}} \exp\left[-\frac{1}{T} H(\omega)\right]}$$

temperature

$A \in \mathcal{B}(\Omega_N)$

partition function

Q: $\tilde{\mathbb{E}}^{a,b,T}[\omega(0)] = ?$

How long is string of 1's around 0?

large N

Need to Simulate

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

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

Background: Detailed Balance & Reversibility

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

trivially true for $i=j$

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

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 & π are in detailed balance. Use fact that Λ consists of "neighboring" sites

For $m \in \Lambda$, $\omega \overset{m}{\sim} \omega'$ if $\omega(n) = \omega'(n)$ for all $n \neq m$.

in Ω

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

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

Start at $\omega \in \Omega$

① Pick an m (equal probabilities: $\frac{1}{2N+1}$)

② Change ω_m to $-\omega_m$ with

$$\underbrace{\omega' = (\omega_{-N} \cdots -\omega_m \cdots \omega_N)}_{S}$$

Probability

$$\frac{\pi(\omega) \wedge \pi(\omega')}{\pi(\omega)} = \underbrace{\frac{\exp\left(-\frac{1}{T} H(\omega)\right) \wedge \exp\left(-\frac{1}{T} H(\omega')\right)}{\exp\left[-\frac{1}{T} H(\omega)\right]}}_{\text{don't need partition function}}$$

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

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

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

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

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 mth site.

Then if $\omega \overset{m}{\sim} \omega'$ 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 $\omega \overset{m}{\sim} \omega'$ for some m,

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

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

- If $\omega \overset{m}{\not\sim} \omega'$ 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

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

should be symmetric in ω & ω'.

Then

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

When $L \geq 1$, we should have a way of picking how we want to change the nth site.

Start at $\omega \in \Omega$

(1) Randomly pick site m (equal probabilities of $\frac{1}{2N+1}$

(2) Randomly pick (equal probabilities)

$W \in \{-L, \ldots, L\} \setminus \{\omega_m\}$.

$$\tilde{\omega} = \begin{cases} \omega_n & \text{if } n \neq m \\ W & \text{if } n = m \end{cases}$$

Metropolis Algorithm

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

$$P_{\omega\tilde{\omega}} = \underbrace{\frac{1}{2N+1}}_{\text{site}} \underbrace{\frac{1}{2L}}_{\text{ways to flip}} \underbrace{\left\{1 \wedge \frac{\pi_{\tilde{\omega}}}{\pi_\omega}\right\}}_{\text{acceptance prob.}} \quad \text{if}$$

$P_{\omega\tilde{\omega}} = 0$ if $\omega \overset{m}{\not\sim} \tilde{\omega}$ for all m

$$P_{\omega\omega} = 1 - \sum_{\substack{m \\ \omega \overset{m}{\sim} \omega'}} P_{\omega\omega'}$$

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

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

Another way

① Randomly pick site m (equal probabilities of $\frac{1}{2N+1}$

② Pick a way to flip m^{th} coordinate with likelihoods

$$\mathbb{P}\{\omega'\} = \frac{\pi_{\omega'}}{\underbrace{\sum_{\omega'' \overset{m}{\sim} \omega} \pi_{\omega''}}_{C_m(\omega)}}$$

Gibbs sampler

$$P_{\omega\tilde{\omega}} = \frac{\overset{\text{site}}{1}}{2N+1} \; \overset{\text{way to flip}}{\frac{\pi_{\tilde{\omega}}}{C_m(\omega)}}$$

$$P_{\omega\tilde{\omega}} = 0 \quad \text{if} \quad \omega \overset{m}{\not\sim} \tilde{\omega} \text{ for all } m$$

$$P_{\omega\omega} = 1 - \sum_{\substack{m \\ \omega \overset{m}{\sim} \omega'}} P_{\omega\omega'}$$

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

$= C_m(\tilde{\omega})$