2/22/2010

Markov Chain Monte Carlo (MCMC)

Metropolis & Glauber

Metropolis Chain

Suppose ψ is a symmetric transition matrix.. Suppose that we censor the chain

modification

$$x \xrightarrow{a(x,y)\,\psi(x,y)} y$$

Can we choose a so that π is steady state?

We get a reversible chain: We want

$$\pi(x)\,\psi(x,y)\,a(x,y) = \pi(y)\,\psi(y,x)\,a(y,x)$$

[If we can achieve ↑, then we get a reversible chain with steady state π]

Since $\psi(x,y) = \psi(y,x)$

$$\Rightarrow \quad b(x,y) = \pi(x)\,a(x,y) = b(y,x)$$

$$\Rightarrow \quad b(x,y) \le \min\{\pi(x), \pi(y)\}$$

We want large a so that we don't spend a lot @ time doing nothing.

Take

$$b(x,y) = \min(\pi(x), \pi(y))$$

and

$$a(x,y) = \min\left\{1, \frac{\pi(y)}{\pi(x)}\right\}$$

Check detailed balance: $b(x,y) = b(y,x)$

$$\min\{\pi(x), \pi(y)\} = \min\{\pi(y), \pi(x)\}$$

✓

Powerful.

Problem is convergence rate.

Remark: chain depends on $\frac{\pi(x)}{\pi(y)}$.

Often we only know that

$$\pi(x) = \frac{h(x)}{Z}$$

Partition Function

We know h, but not Z.

$$\frac{\pi(x)}{\pi(y)} = \frac{h(x)}{h(y)}$$ and we are O.K.

Rem 3.2

Optimization: Suppose we want to maximise $f(x)$, $x \in \Omega$ $\qquad f > 0$.

$$\pi_\lambda(x) = \frac{\lambda^{f(x)}}{Z(\lambda)} \qquad Z(\lambda) = \sum_x \lambda^{f(x)}$$

If $\Omega^* = \{ x \in \Omega : f(x) = f^* = \max_x f(x) \}$

$$\lim_{\lambda \to \infty} \pi_\lambda(x) = \lim_{\lambda \to \infty} \frac{\lambda^{f(x)} / \lambda^{f^*}}{|\Omega^*| + \sum_{x \notin \Omega^*} \lambda^{f(x)} / \lambda^{f^*}} = \frac{1_{\{x \in \Omega^*\}}}{|\Omega^*|}.$$

General ψ (not nec. symmetric)

$$a(x,y) = \min\left\{ \frac{\pi(y)\,\psi(y,x)}{\pi(x)\,\psi(x,y)},\ 1 \right\}$$

Check

$$\pi(x)\,\psi(x,y)\,a(x,y) = \min\left\{ \pi(y)\,\psi(y,x),\ \pi(x)\,\psi(x,y) \right\}$$

Example

Random walk on a graph:

$$\psi(x,y) = \frac{1}{\deg(x)} \qquad y \in N(x)$$

$$a(x,y) = \min\left\{1, \frac{\deg(x)}{\deg(y)}\right\} \qquad \frac{\pi(x)}{\pi(y)}$$

Steady state is uniform

Glauber Dynamics

Context: $\Omega \subseteq S^V$ $\{$configurations$\}$

$\sigma \in \Omega$: each $v \in V$ has a <u>spin</u> $\sigma(v)$.

<u>Ex 1</u>: $G = (V, E)$

$S = \{1, 2, \dots, q\}$

$\Omega = \{$ proper colorings $\}$

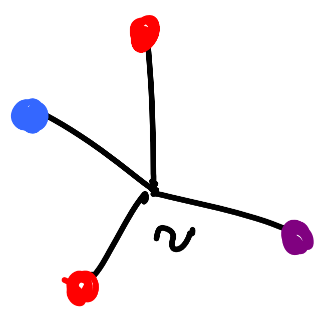
Glauber: $X_0, X_1, \ldots X_t, \ldots \in \Omega$

X_t = a proper coloring of G.

Chain:

(i) Choose $v \in V$ uniformly at random

(ii) $A_v(X_t)$ $= \{ c : X_t(w) \neq c, \forall w \in N_G(v) \}$



(iii) Choose c uniformly from $A_v(X_t)$

(iv) $X_{t+1}(w) = \begin{cases} c : & w = v \\ X_t(w) : & w \neq v \end{cases}$

Steady State: $\sigma, \tau \in \Omega$

$$P(\sigma,\tau) = \begin{cases} |V|^{-1} \times |A_v(\sigma)|^{-1} & h(\sigma,\tau) = 1 \ \& \ \sigma(v) \neq \tau(v) \\ 0 & \end{cases}$$

$$= P(\tau, \sigma)$$

$A_v(\sigma) = A_v(\tau)$

determined by colors at

$N_G(v)$

Detailed Balance

says that steady state is uniform

Ex2 : $\Omega = \{ \text{independent sets of } G \}$

2 spins 0 & 1

1 & 1 ← forbidden

1

Hard Core Model

Glauber : (i) Choose v uniformly at random

(ii) If $N(v) \cap X_t = \emptyset$

then $X_{t+1} = X_t \cup \{v\}$ Prob $1/2$

$= X_t$ Prob $1/2$

Uniform Steady State

General Description

$\Omega \subseteq S^V$

π is target stationary distribution

$x \in \Omega$, $v \in V$

$$\Omega(x,v) = \{ y \in \Omega : y(w) = x(w), \ w \neq v \}$$

$$P(x,y) = \begin{cases} \dfrac{\pi(y)}{\pi(\Omega(x,v))} \cdot \dfrac{1}{|V|} & : \ y \in \Omega(x,v) \\ 0 & : \ \text{otherwise} \end{cases}$$

$$\pi(x) P(x,y) = \frac{\pi(x)\pi(y)}{|V| \pi(\Omega(x,v))} \quad \forall P(x,y) > 0$$

Hard core with fugacity

$$\Omega = \{\text{independent sets}\} \qquad \lambda > 0$$

fugacity

$$\pi(I) = \frac{\lambda^{|I|}}{\sum_{I \in \Omega} \lambda^{|I|}}$$

$X_t = x$: choose v randomly

$$X_{t+1}(v) = \begin{cases} 1 & : \frac{\lambda}{1+\lambda} \\ 0 & : \frac{1}{1+\lambda} \end{cases}$$

$N_v(X_t) = \emptyset$

$$\frac{\lambda}{1+\lambda} = \frac{\lambda^{a+1}}{\lambda^a + \lambda^{a+1}}$$

a = #1's outside v

Ising

Magnets

$$\Omega = \{-1, 1\}^V$$

For $\sigma \in \Omega$, $H(\sigma) = -\sum_{(v,w)\in E} \sigma(v)\,\sigma(w)$

Hamiltonian
(Energy)

$$\mu(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z(\beta)} \quad \text{where } Z(\beta) = \sum_{\sigma} e^{-\beta H(\sigma)}$$

$\beta \geq 0$

$\frac{1}{\text{Temperature}}$

μ : target distribution

Glauber: σ, τ differ at v

$$P(\sigma,\tau) = \frac{1}{|V|} \cdot \frac{e^{\beta S(\sigma,\tau)}}{e^{\beta S(\sigma,\tau)} + e^{-\beta S(\sigma,\tau)}}$$

$\tau(v) = +1$

where $$S(\sigma,\tau) = \sum_{w \in N_\sigma(v)} \sigma(w)$$