Markov Chain Monte Carlo (MCMC)
Metropolis & Glauber

Suppose $\psi$ is a symmetric transition matrix. Suppose that we censor the chain modification $a(x,y)\psi(x,y)$.

Can we choose $a$ so that $\pi$ is a 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 \( \uparrow \), then we get a reversible chain with steady state \( \frac{\Pi}{\max} \)]

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

\( \Rightarrow \)

\( b(x, y) = \Pi(x) a(x, y) = b(y, x) \)

\( \Rightarrow \)

\( b(x, y) \leq \min \left\{ \frac{\Pi(x)}{\Pi(y)} \right\} \)

We want large \( A \) so that we don't spend a lot of time doing nothing.
Take

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

and

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

Check detailed balance: $b(x, y) \leq b(y, x)$

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

√

Powerful.

Problem in convergence rate.
Remark: Chain depends on $\frac{\pi(2x)}{\pi(1)}$.

Often we only know that

$$\frac{\pi(2x)}{\pi(1)} = \frac{h(x)}{Z}$$

We know $h$, but not $Z$.

$\Pi Z = h(x)$ and we are O.K.
Optimization: Suppose we want to maximize $f(x)$, $x \in \mathbb{R}$, $f > 0$.

$$
\overline{n}_\lambda (x) = \frac{\lambda f(x)}{Z(\lambda)}
$$

$$
Z(\lambda) = \sum_x \lambda f(x)
$$

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

$$
\lim_{\lambda \to \infty} \overline{n}_\lambda (x) = \lim_{\lambda \to \infty} \frac{\lambda f(x)/f^*}{1 + \sum_{x \in \Omega^*} \lambda f(x)/f^*} = \frac{1}{f(x)/f^*}.
$$
General $\Psi$ (not necessarily 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:

\[ \psi(x, y) = \frac{1}{\deg(x)} \]

\[ \alpha(x, y) = \min \left\{ \frac{\deg(x)}{\deg(y)} \right\} \]

\[ y \in N(x) \]

Steady state is uniform
Glauber Dynamics

Context: $\Omega \subseteq \mathcal{S}$ \{configurations\}

$\sigma \in \Omega$: each $v \in V$ has a spin $\sigma(v)$.

Ex 1: $G = (V, E)$

$\mathcal{S} = \{1, 2, \ldots, q\}$

$\Omega = \{\text{proper colorings}\}$
Glauber: $X_0, X_1, \ldots, X_t, \ldots \in \Omega$

$X_t$: a proper coloring of $G$.

Chain:
1) Choose $v \in V$ uniformly at random
2) $A_v(X_t) = \{ c : X_v(w) = c, \forall w \in N_G(v) \}$

3) Choose $c$ uniformly from $A_v(X_t)$
4) $X_{t+1}(w) = \begin{cases} c : w = v \\ X_t(w) : w \neq v \end{cases}$
Steady State: \( \sigma, T \in \mathcal{Q} \)

\[
P(\sigma, T) = \begin{cases} 
|V|^{-1} \times |A_{\nu}(\alpha)|^{-1} & h(\sigma, T) = 1 \\
0 & \sigma(\nu) \neq \tau(\nu)
\end{cases}
\]

\[= P(\tau, \sigma) \]

A\textcolor[rgb]{1.00,1.00,0.00}{\nu}(\alpha) < A\textcolor{green}{\nu}(\alpha)
determined by colors at \( N_{\alpha}(\nu) \)

Detailed Balance says that steady state is uniform
Ex 2: $\Omega = \xi$ independent satisfying $G\xi$

2 spins 0 & 1

Hard Core Model

Glauber: (i) Choose $\omega$ uniformly at random

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

then $X_{t+1} = X_t \cup \{\omega\}$

$P_{\omega} = \frac{1}{2}$

$P_t = \frac{1}{2}$

Uniform Steady State
General Description

\[ \Omega \subseteq \mathbb{S}^n \]

\( \Pi \) is a target stationary distribution

\( x \in \Omega, \ \forall \nu \in \mathbb{N} \)

\[ \Omega(\omega, \nu) = \{ y \in \Omega : y(\omega) = x(\omega), \ \nu + 1 \} \]

\[ P(x, y) = \begin{cases} \frac{\Pi(y)}{\Pi(x, \nu)} \cdot \frac{1}{|\nu|} & : y \in \Omega(\nu, \nu) \\ 0 & : \text{otherwise} \end{cases} \]
\[ \prod \lambda^{1_{\mathcal{I}}} \geq \frac{\prod \lambda^{1_{\mathcal{I}}}}{\prod \lambda^{1_{\mathcal{I}}}} \]

\[ \text{Hard core with fugacity} \]

\[ \Omega = \frac{1}{2} \text{ independent set s.t. } \lambda > 0 \]

\[ \lambda = \frac{\lambda^{a_{i}+}}{\lambda^{a_{i}}} \]

\[ X_t = \text{choose } v \text{ randomly} \]

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

\[ N_{x_{t}}(X_{t}) = 0 \]
Ising
\[ \Omega = \{ -1, 1 \}^V \]

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

\[ Z(\beta) \]

where \( Z(\beta) = \sum_{\sigma} e^{-\beta H(\sigma)} \)

\[ \mu(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z(\beta)} \]

\( \beta > 0 \)

Temperature

Magnetic
Glauber: \( \sigma \), \( \tau \) differ at \( \nu \)

\[
\rho(\sigma, \tau) = \frac{1}{2N} \cdot \frac{e^{\beta S(\sigma, \tau)}}{e^{\beta S(\sigma, \tau)} + e^{-\beta S(\sigma, \tau)}}
\]

\( \tau(\nu) = +1 \)

where \( S(\sigma, \tau) = \sum_{\nu \in \Omega} \sigma(\nu) \)