Reversible MC

Def Let \((X_0, X_1, \ldots)\) be a M.C. with state space \(E\) and transition matrix \(P\). A probability dist. \(\pi\) on \(E\) is said to be reversible for the chain (or for the transition matrix \(P\)) if \(\pi_j P_{ij} = \pi_i P_{ij}\) for all \(i, j\) we have

\[\pi_i P_{ij} = \pi_j P_{ij}\]

A Markov C. is said to be reversible if it has a reversible distribution.

Thm Let \((X_n)\) be a M.C. with state space \(E\) and transition matrix \(P\). If \(\pi\) is a reversible dist. for the chain, then it is also a stationary dist. for the chain.

proof We have to show that \(\forall j\)

\[\pi_j = \sum_i \pi_i P_{ij}\]

\[\pi_j = \pi_j \sum_i P_{ji} = \pi_j \sum_i \pi_i P_{ij}\]

\[\pi_j = \sum_i \pi_i P_{ij}\]
**Ex: Random Walk on graphs**

Graph: $G = (V, E)$

$V = \{v_1, \ldots, v_k\}$ vertex set

$E = \{e_1, \ldots, e_l\}$ edge set

Two vertices are said to be neighbors if they share an edge.

$cl_i$ : # of neighbors of vertex $i$

$P_{i,j} = \begin{cases} \frac{1}{cl_i} & \text{if } v_i \text{ and } v_j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases}$

$\pi = \left( \frac{d_1}{cl_1}, \ldots, \frac{d_k}{cl_k} \right)$

$cl = \sum_{i=1}^{k} d_i$

$\pi_i P_{i,j} = \frac{d_i}{cl} \frac{1}{d_j} = \frac{d_j}{cl} \frac{1}{d_j} = \pi_j P_{j,i}$

$\pi = \left( \frac{2}{24}, \frac{3}{24}, \frac{5}{24}, \frac{3}{24}, \frac{2}{24}, \frac{3}{24}, \frac{3}{24}, \frac{3}{24} \right)$

**Ex: king on chessboard. The M.C. is irreducible &aperiodic. inv. dist. $\pi$ , compute $\pi$**
Ex Time reversal

Let $(X_0, X_1, \ldots)$ be a reversible M.C. with state space $E$, transition matrix $P$, and reversible drift $\pi$.

Show that if the chain is started with initial distribution $\mu^n = \pi$, then $\forall n$ and $\forall i_0, \ldots, i_n$ in $E$ we have

$$P(\{X_0 = i_0, X_1 = i_1, \ldots, X_n = i_n\}) = P(\{X_0 = i_n, \ldots, X_n = i_0\})$$

In other words, the chain is equally likely to make a tour through the states $i_0, \ldots, i_n$ in both forward or backwards order.

Ex 2 Birth and death process

\[ \begin{array}{cccccc}
1 & \rightarrow & 2 & \rightarrow & 3 & \rightarrow & \cdots & \rightarrow & k \\
\end{array} \]

$(X_0, X_1, \ldots)$ M.C. with state space $E = \{1, \ldots, k\}$

(i) $P_{ij} > 0$ whenever $|i - j| = 1$

(ii) $P_{ij} = 0$ whenever $|i - j| > 1$

Find $\pi$
Look for a reversible chain.

Take $\pi_i : a > 0$

Condition $\pi_i p_{ij} = \pi_j p_{ji} \Rightarrow$

$$\pi_i^k = \frac{a p_{ik}}{p_{ii}}$$

$$\pi_i^k = \pi_i^k \frac{p_{ij}}{p_{ji}} = \frac{a p_{ik} p_{ij}}{p_{ii} p_{ji}}$$

$$\pi_i^k = \frac{\prod_{j \neq i}^{i} p_{ej}}{\pi_{i}, e}$$

$$\prod_{i=1}^{n} \pi_i^{*} = \frac{\prod_{i=1}^{n} p_{ei}}{\sum_{e=1}^{n} \pi_e^{*}}$$
Simulation by Markov Chains

\[ E : \text{finite state space} \]
\[ \pi \in \mathcal{P}(E) \]
\[ \rho : E \to \mathbb{R} \]

We want to compute

\[ E_\pi \left[ \rho \right] = \sum_{\pi \in E} \rho(\pi) \pi(\pi) \]

or sample a state \( \pi \in E \) under the law \( \pi \)

Ex: The hard-core model

Let \( G = (V, E) \) be a graph

- vertex set: \( V = \{ v_1, \ldots, v_k \} \)
- edge set: \( E = \{ e_1, \ldots, e_l \} \)

A hard-core configuration on \( G \) is a finite sequence

\[ \chi = (\chi(v))_{v \in V} \in \{0,1\}^V \]

such that \( \chi(v_1) \chi(v_2) = 0 \) if \( v_1 \) and \( v_2 \) share an edge

Interpretation:
- 1 \( \rightarrow \) particles of non negligible radii
- 0 \( \rightarrow \) empty locations
Let \( E \subset \{0,1\}^V \) be the set of all hard core configurations.

and \( \pi \) the uniform probability on \( E \).

Compute: \( \mathbb{E}_\pi \left[ \sum_{v \in V} x(v) \right] \); expected \# of occupied sites under \( \pi \)

\[
\begin{array}{c}
\text{8x8 grid} \\
\text{Card}(\{0,1\}^V) = 2^64
\end{array}
\]

Solution: \( E, \pi \)

Find a transition matrix \( P \) on \( E \) (irreducible, aperiodic)

such that \( \pi \) is the invariant dist. of \( P \).

Generate (simulate) the M.C. \((X_0, X_1, \ldots)\) associated to \( P \).

The law of \( X_0 \) can be anything (uniform or dirac mss)

then

\[
\frac{1}{N} \sum_{i=1}^{N} p(X_i) \overset{\text{o.s.}}{\rightarrow} \mathbb{E}_\pi [p]
\]

\( \text{Chernoff bound: } P \left[ | S_N - \mathbb{E}_\pi [p] | \geq \varepsilon \right] \leq C e^{-c \varepsilon^2 N} \)
Metropolis Algorithm

⇒ produce a reversible M.C. with respect to $\pi$

⇒ Let $Q$ be a stochastic matrix on $E$ (called selection matrix) such that $\forall (x, y) \in E \times E$

\[ Q(x, y) > 0 \Rightarrow Q(y, x) > 0 \]

Let $h: [0, \infty) \rightarrow [0, 1]$ a function satisfying

\[ h(u) = u h\left(\frac{1}{u}\right) \]

\[ e_x h(u) = \inf_{0 < u < e_x} (u, 1) \]

or \[ h(u) = \frac{u}{1 + u} \]

For $x \neq y$ write

\[ R(x, y) = \begin{cases} h\left(\frac{\pi(y)}{\pi(x)} \frac{Q(y, x)}{Q(x, y)}\right) & \text{if } Q(x, y) \neq 0 \\ 0 & \text{otherwise} \end{cases} \]

Define $P$ by

\[ P(x, y) = Q(x, y) R(x, y) \quad \text{for } x \neq y \]

and

\[ P(x, x) = 1 - \sum_{y \neq x} P(x, y) \]
Thm Assume that \( \forall x \in E, \pi(x) > 0 \)

P is reversible with respect to \( \pi \). It is irreducible if \( Q \) is irreducible. Moreover, if \( h(w) < 1 \) (for instance \( h(w) = \frac{w}{1+w} \)) then it is aperiodic.

\[
\begin{align*}
\text{proof} & \quad \pi(x) P(x, y) = \frac{\pi(x) Q(x, y)}{\pi(y) Q(y, x)} h \left( \frac{\pi(y) Q(y, x)}{\pi(x) Q(x, y)} \right) \\
& = h \left( \frac{\pi(x) Q(x, y)}{\pi(y) Q(y, x)} \right) \pi(y) Q(y, x) \\
& = P(y, x) \pi(y)
\end{align*}
\]
Metropolis Algorithm

Step 0: Initialize $X_0$

Step n+1: Choose $y \in E$ with the law $Q(X_n, y)$

choose $U$ at random uniformly in [0,1]

If $U < R(X_n, y)$ accept the selection

$X_{n+1} = y$

If not, refuse the selection

$X_{n+1} = X_n$

produce a MC with transition matrix $P$
Hard Core Model

Step 0: \( X_0 (v) = 0 \) \( \forall v \in V \)

Step 1:
1. Choose \( v \in V \) at random (uniformly)
2. Toss a fair coin
3. If the coin comes up \( H \) and all the neighbors of \( v \) take value 0 in \( X_0 \) then let \( X_{n+1} (v) = 1 \); otherwise let \( X_{n+1} (v) = 0 \)
4. \( \forall w \neq v \), let \( X_{n+1} (w) = X_n (w) \)

Ex: Check that the previous algorithm is a Metropolis algorithm

\[
h(v) = \frac{v}{1 + v} \quad (\Rightarrow R(x, y) = \frac{1}{v} \text{ if } \Phi(x, y) = 0) \]

\( Q : E \times E \rightarrow [0, 1] \)

defined by \( Q(x, y) = \frac{1}{\text{corel}(V)} \) if \( x \) and \( y \) differ at only one site

and \( Q(x, y) = 0 \) if \( x \) and \( y \) differ at at least 2 sites
Generalized hard core model

\( G = (V, E) \)

\( x = x(v), v \in V \in \{0, 1\}^V \)

Let \( \lambda > 0 \)

\( \mu \in \mathcal{B}(\{0, 1\}^V) \)

\[ \mu_G, \lambda (x) = \begin{cases} \lambda^{n(x)} & \text{if } x \text{ is a hard core configuration} \\ \frac{1}{Z_G, \lambda} & \text{otherwise} \end{cases} \]

\[ n(x) = \sum_{v \in V} x(v) \]

\[ Z_{G, \lambda} = \sum_{x \in \{0, 1\}^V} \lambda^{n(x)} \text{ if } x \text{ is a hard core configuration} \]

\[ \Rightarrow \mu_G, \lambda (v = 1 \mid w = 0 \text{ for a } (w,v) \in E) = \frac{\lambda}{\lambda+1} \]

\[ \mu_G, \lambda (v = 1 \mid \exists w, (w,v) \in E, w = 1) = 0 \]

\( \lambda = 1 \) is a standard hard core model

Construct an MCMC algorithm for this generalized hard core model.
Q: $E \times E \rightarrow [0,1]$

$Q(x, y) = \frac{1}{\text{card}(V)}$ if $(x, y)$ differ at only one site

$Q(x, y) = 0$ if $(x, y)$ differ at at least 2 sites

$h(u) = \frac{u}{1+u}$

$R(x, y) = \begin{cases} h\left(\frac{\pi(y)Q(x, y, x)}{\pi(x)Q(x, y)}\right) & \text{if } Q(x, y) \neq 0 \\ 0 & \text{otherwise} \end{cases}$

$P(x, y) = Q(x, y)R(x, y)$ for $x \neq y$

$P(x, x) = 1 - \sum_{y \neq x} P(x, y)$

$\pi(x) = \bigvee_{G, \lambda} \lambda(x)$

$\frac{\pi(y)}{\pi(x)} = \begin{cases} \lambda & \text{if } \eta(y) - \eta(x) = 1 \\ \frac{1}{\lambda} & \text{if } \eta(y) - \eta(x) = -1 \end{cases}$

$h\left(\frac{\pi(y)Q(x, y, x)}{\pi(x)Q(x, y)}\right) = \begin{cases} \frac{\lambda}{1+\lambda} & \text{if } \eta(y) - \eta(x) = 1 \\ \frac{1}{1+\lambda} & \text{if } \eta(y) - \eta(x) = -1 \end{cases}$
MCMC algorithm for (random) $q$-coloring

Graph $G = (V, E)$

$q \in \mathbb{N}, \ q \geq 2$

A $q$-coloring of $G$ is a finite sequence

$\chi = (\chi(u))_{u \in V} \in \{1, \ldots, q\}^V$

colors

with the property that no two adjacent vertices have the same value (color)

Rk Existence of a $q$-coloring not obvious

Thm If $G$ is planar, then there exists

$q$-coloring of $G$ for $q \geq 4$

Random $q$-coloring: a $q$-coloring chosen uniformly from
the set of possible $q$-colorings of $G$

$\mathcal{P}_{q}^G$: corresponding prob. dist. on $\{1, \ldots, q\}^V$

Find a M.C. with stat. dist. $\mathcal{P}_{q}^G$
Step \( n \rightarrow n+1 \)

1. Pick a vertex \( v \in V \) at random (uniformly)

2. Pick \( X_{n+1}(v) \) according to the uniform
class over the set of colors that are not
attained by any neighbor of \( v \)

3. Leave the color unchanged at all vertices
i.e. let \( X_{n+1}(w) = X_n(w) \) \( \forall w \in V \), except \( v \)

Chain isaperiodic and has \( \rho \) as
state dist.

irreducibility: hard question