

# Markov chain Monte Carlo (MCMC)

One goal (as before): Estimate  $\mu = E_{\pi}(g(x))$

where expectation is difficult/impossible to do analytically.

~~Most~~ Often:

Cannot use iid Monte Carlo since we are unable to simulate  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \pi$ .

Can use imp. sampling in principle but if  $\pi$  is complicated, difficult to find good importance function, especially as dimensions increase.

MCMC solution: Construct <sup>a Harris ergodic</sup> Markov chain

$\underline{X} = (X_1, X_2, \dots)$  s.t. it has stationary distribution

$\pi$ . Simulate  $X_1, X_2, X_3, \dots, X_n$  and,

obtain estimate  $\hat{\mu}_n = \frac{\sum_{i=1}^n g(X_i)}{n}$ .

Under similar conditions to iid. case, we can appeal to S.L.L.N.  $\hat{\mu}_n \rightarrow \mu$ .

Conditions for a C.L.T. are more ~~diff~~ complicated.

Note: Importance sampling and MCMC are not mutually exclusive. Can reweight dependent samples above and obtain importance sampling estimators. E.g. tail probabilities, max. likelihood, multiple expectations w/ a single set of samples etc

Metropolis-Hastings algorithm.

Algorithm used to construct a Harris ergodic chain w/ stationary distr.  $\pi(x)$ ,  $x \in \Omega$

Let transition kernel,  $K(x, y)$ , be a generalization of a transition probability matrix,  $P_{xy}$  or  $P(x, y)$ .  
( $P_{ij}$  before)

As w/ tpm, transition kernel specifies conditional probabilities, i.e.,  $K(x, y) = k(y|x)$ , where  $k(y|x)$  is a pdf when  $x, y$  are states in a continuous state space M.Chain.

We want  $K(x, y)$  to satisfy detailed balance w.r.t.  $\pi$ :

$$\pi(x) K(x, y) = \pi(y) K(y, x).$$

We specify such a  $K(x, y)$  using the Metropolis-Hastings algorithm: Define  $h(x)$  s.t.  $\pi(x) = h(x)/c$

Start w/  $X_0 = x_0 \in \Omega$ . For  $n = 0, 1, 2, \dots$

If  $X_n = x$ ,  $X_{n+1}$  is generated as follows:

- ① Generate a candidate or proposal  $y \sim q(x, y)$ , where  $q(x, y)$  is really  $q(y|x)$  so proposal  $y$  may depend on current value  $x$ . For cntr state space,  $q(y|x)$  is just a conditional pdf.
- ② Set  $X_{n+1} = y$  (accept proposal  $y$ ) w/ probability  
$$\alpha(x, y) = \begin{cases} \min\left(\frac{h(y) q(y, x)}{h(x) q(x, y)}, 1\right) & \text{if } \pi(x) q(x, y) > 0 \\ 1 & \text{else} \end{cases}$$
  
else reject proposal  $y$  and set  $X_{n+1} = x$ .

Requirements on  $q$ :

- (a)  $q(x, y) = 0 \Rightarrow q(y, x) = 0 \quad \forall x, y \in \Omega$
- (b)  $q(x, y)$  is transition kernel of irreducible M.C.

$X_0, X_1, X_2, \dots$  is an M.C., Harris ergodic, w/  
stationary distr.  $\pi$ .

E.g. Observe  $Y_1, \dots, Y_n$

Model:  $Y_i | \theta \sim N(\theta, 1)$  conditl. indep.

$\theta \sim \text{Log-t}(\mu, \sigma, r)$

Want posterior distr. of  $\theta$ :

$$\pi(\theta | \underline{y}) \propto \mathcal{L}(\underline{y} | \theta) p(\theta)$$
$$= \prod_{i=1}^n \frac{1}{\sqrt{2\pi}} \exp \left\{ -\frac{1}{2} (Y_i - \theta)^2 \right\} \times \frac{1}{\theta} \left[ 1 + \frac{1}{r} \left( \frac{\log \theta - \mu}{\sigma} \right)^2 \right]^{-\frac{(r+1)}{2}}$$

$$\propto \frac{1}{\theta} \exp \left\{ -\frac{1}{2} \sum_{i=1}^n (Y_i - \theta)^2 \right\} \times \left[ 1 + \frac{1}{r} \left( \frac{\log \theta - \mu}{\sigma} \right)^2 \right]^{-(r+1)/2}$$

Suppose we choose to sample from  $\pi(\theta | \underline{y})$  by  
Metropolis-Hastings and let  $\pi(\theta | \underline{y}) = h(\theta)/c$  where  $c$

is unknown normalizing constant.

$$h(\theta) = \frac{1}{\theta} \exp \left\{ -\frac{1}{2} \sum_{i=1}^n (Y_i - \theta)^2 \right\} \times \left[ 1 + \frac{1}{r} \left( \frac{\log \theta - \mu}{\sigma} \right)^2 \right]^{-(r+1)/2}$$

We now need to find proposal  $q$ .

The Metropolis algorithm ('random walk' Metropolis-Hastings)

M-H algorithm where  $q(x,y) = q(y,x)$  for all  $x,y$ .

That is, M-H algorithm w/ symmetric proposal, so

$$\text{acceptance prob. } \alpha(x,y) = \min \left\{ 1, \frac{\pi(y)}{\pi(x)} \frac{q(y,x)}{q(x,y)} \right\}$$
$$= \min \left\{ 1, \frac{\pi(y)}{\pi(x)} \right\}$$

E.g.  $q(x,y)$  is a normal density centered at  $x$ .

Propose new value  $y^* \sim q(x, \cdot)$  so  $y^* \sim N(x, \tau^2)$

Variance  $\tau^2$  is a tuning parameter: affects how well the algorithm performs.

$\tau^2$  too big: candidates generated far from current value, maybe in tails  $\Rightarrow$  low prob. of being accepted.

$\tau^2$  too small: proposals/candidates accepted often but too close to previous value  $\Rightarrow$  chain explores state space very slowly and high autocorrelations across sampled values (large variance / M-error)

# Metropolis-Hastings : some history

1940s: Monte Carlo invented by physicists working in Los Alamos: S. Ulam, J. von Neumann, N. Metropolis  
Metropolis and Ulam (1949) JASA:  
1953: Metropolis, Rosenbluth, Teller<sup>2</sup> (J. Chem. Phys.) Los Alamos  
Natl. Labs

1970: Hastings (Biometrika) rediscovered, generalized

1984: Geman & Geman Gibbs distr. used in image analysis

1987: Tanner & Wong (JASA) Data augmentation alg.

1990: Gelfand & Smith (JASA) Used in Bayesian inference  
Gibbs sampler

1994: Tierney (Annals) Laid out all theory

1995: Green (Biometrika): Dimension-jumping  
reversible-jump M-H alg.

All fall under umbrella of M-H algorithm

Return to our example. Want to simulate from  $\pi(\theta|y)$ .

Suppose we use Metropolis algorithm.

$q(\theta, \theta^*)$  is  $N(\theta, \tau^2)$ . Symmetric since  $q(\theta, \theta^*) = q(\theta^*, \theta)$ .

Algorithm: When current value of M-chain, say,  $\theta^{(n)} = \theta$ , propose new value  $\theta^* \sim N(\theta, \tau^2)$ .

Accept  $\theta^*$  w/ prob.  $\alpha(\theta, \theta^*) = \min \left\{ 1, \frac{\pi(\theta^*)}{\pi(\theta)} \right\}$   
 $= \min \left\{ 1, \frac{h(\theta^*)}{h(\theta)} \right\}$

M-H recipe:

Start M.C. at  $\theta^{(0)} = c$  for some  $c > 0$ .

For  $i = 1, \dots, n$

Propose  $\theta^* \sim N(\theta^{(i-1)}, \tau^2)$

Accept  $\theta^*$  w/ probability  $\alpha(\theta^{(i-1)}, \theta^*) = \min \left\{ 1, \frac{h(\theta^*)}{h(\theta^{(i-1)})} \right\}$   
i.e.,  $\theta^{(i)} = \theta^*$   
else reject, i.e.,  $\theta^{(i)} = \theta^{(i-1)}$

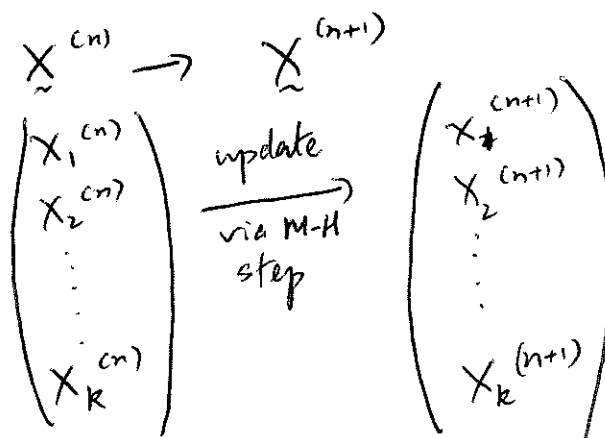
For any expectation <sup>that exists,</sup>  $M = E_{\pi} \{g(\theta)\}$  can obtain an estimate  $\hat{M}_n = \frac{\sum_{i=1}^n g(\theta^{(i)})}{n}$ .

$\therefore \hat{M}_n \xrightarrow{P} M$  as  $n \rightarrow \infty$

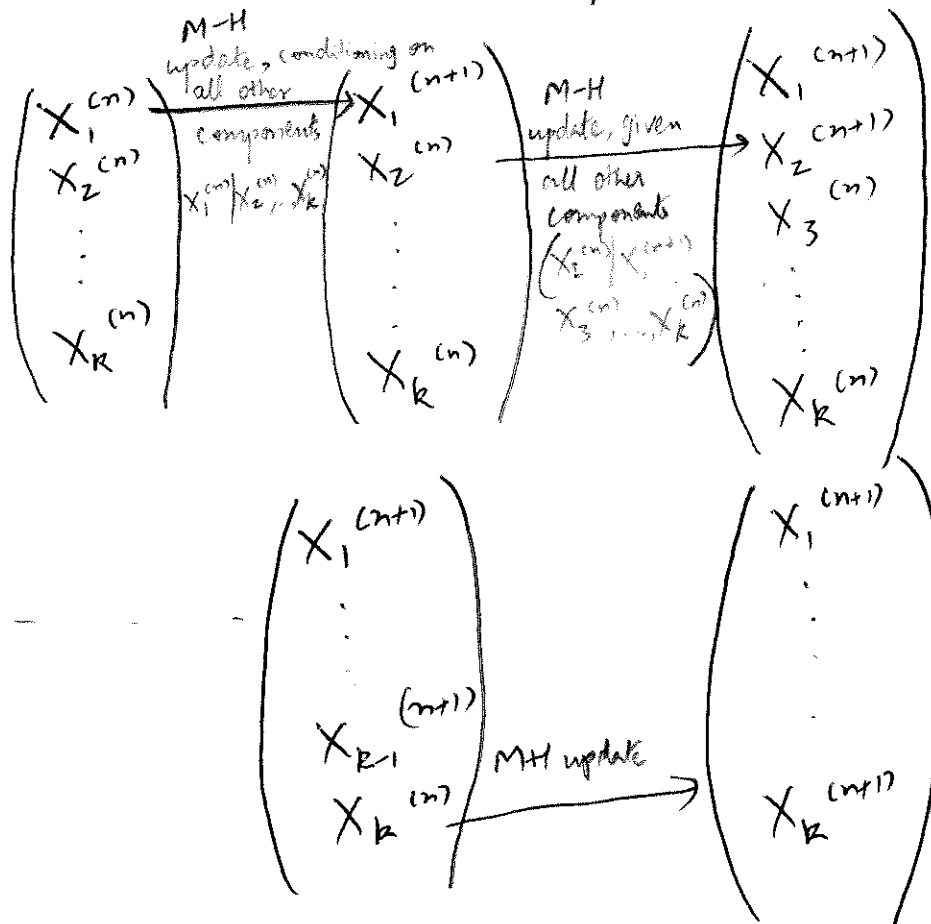
# Variable-at-a-time M-H: (for multivariate distr.)

Main idea: suppose target distr. has  $K$  components.

'All-at-one' M-H alg.  
(already discussed)



Variable-at-a-time M-H:  
 $n^{\text{th}}$  update done in  
small steps



Note: each component may itself be multidimensional.

## Variable-at-a-time M-H:

Finding transition Kernel  $K$  (i.e. proposal  $q$ ) to ~~success~~ efficiently sample from  $\pi$  may be difficult when state space is multidimensional.

Similar issues as importance sampling, rejection sampling:

Instead, apply M-H to sub blocks/components.

E.g. if  $\underline{x} = (x_1, x_2)$

'Full conditl. distr.' of  $x_1 = \pi_{1|2}(x_1 | x_2)$

" " " "  $x_2 = \pi_{2|1}(x_2 | x_1)$

Let  $K_{1|2}(x_1, y_1 | x_2)$  and  $K_{2|1}(x_2, y_2 | x_1)$  be transition kernels w/ stationary distr.  $\pi_{1|2}$  and  $\pi_{2|1}$  respectively.

Two step M-H update:

1. Generate  $x_1^{(n+1)}$  using  $K_{1|2}(x_1^{(n)}, \cdot | x_2^{(n)})$ , M-H update
2. Generate  $x_2^{(n+1)}$  using  $K_{2|1}(x_2^{(n)}, \cdot | x_1^{(n+1)})$ , M-H update

Equivalent to a single update w/ transition kernel

$$K((x_1, x_2), (y_1, y_2)) = \underbrace{K_{1|2}((x_1, y_1) | x_2)}_{\text{update 1st component}} \underbrace{K_{2|1}(x_2, y_2 | y_1)}_{\substack{\text{update 2nd component} \\ \text{given 1st update}}}$$



Example: suppose  $\underline{x} = (x_1, x_2, x_3)$  where each block may ~~also~~ be multidimensional.

Need:  $K_{1|(2,3)}$  w/ stationary distr.  $\overset{\text{full condit.}}{\downarrow} \pi_{1|(2,3)}(x_1|x_2, x_3)$   
 $K_{2|(1,3)}$  " " "  $\pi_{2|(1,3)}(x_2|x_1, x_3)$   
 $K_{3|(1,2)}$  " " "  $\pi_{3|(1,2)}(x_3|x_1, x_2)$

Construct  $K_{1|2,3}, K_{2|1,3}, K_{3|1,2}$  by using M-H alg.  
w/ proposals  $q_1, q_2, q_3$  respectively

If full conditl. distr. is standard distr., can directly sample from it. For e.g. if  $\pi_{1|2,3} = \text{Normal density}$  simulate update for  $x_1$  from a normal.

→ skip below

If current state =  $\underline{x}^{(n)} = (x_1^{(n)}, x_2^{(n)}, x_3^{(n)})$  produce next state =  $\underline{x}^{(n+1)} = (x_1^{(n+1)}, x_2^{(n+1)}, x_3^{(n+1)})$  in 3 steps:

① Propose  $x_1^* \sim q_1(x_1^*, x_1^{(n)} | x_2^{(n)}, x_3^{(n)})$

Accept  $x_1^*$ , ie, set  $x_1^{(n+1)} = x_1^* \neq$  w/ prob.

$$\alpha(x_1^{(n)}, x_1^* | x_2^{(n)}, x_3^{(n)})$$

$$= \min \left\{ 1, \frac{\pi_{1|2,3}(x_1^* | x_2^{(n)}, x_3^{(n)}) q(x_1^{(n)}, x_1^* | x_2^{(n)}, x_3^{(n)})}{\pi_{1|2,3}(x_1^{(n)} | x_2^{(n)}, x_3^{(n)}) q(x_1^*, x_1^{(n)} | x_2^{(n)}, x_3^{(n)})} \right\}$$

else set  $x_1^{(n+1)} = x_1^{(n)}$  (reject  $x_1^*$ ).

(2) Propose  $x_2^* \sim q_2(x_1^{(n)}, x_2^* | \underbrace{x_1^{(n+1)}, x_3^{(n)}}_{\substack{\downarrow \\ \text{(note updated value)}}})$

Accept: Set  $x_2^{(n+1)} = x_2^*$  w/ prob.  $\alpha(x_1^{(n)}, y_2 | x_1^{(n+1)}, x_3^{(n)})$   
 else (Reject):  $x_2^{(n+1)} = x_2^{(n)}$ .

(3) Propose  $y_3 \sim q_3(x_3^{(n)}, x_3^* | x_1^{(n+1)}, x_2^{(n+1)})$   
 Accept: set  $x_3^{(n+1)} = x_3^*$  w/ prob.  $\alpha(x_3^{(n)}, x_3^* | x_1^{(n+1)}, x_2^{(n+1)})$   
 (Reject) else  $x_3^{(n+1)} = x_3^{(n)}$ .

The Markov chain constructed by this algorithm  
 is Harris-ergodic w/ stationary distribution  $\pi$ .

Simple example: Poi-Gamma model

(C & L p. 143)

$$Y_i | \theta_i \sim \text{Poi}(\theta_i t_i) \quad \text{condit. indep.} \quad i=1, \dots, K$$

Prior  $\theta_i | \beta \sim \text{Ga}(\alpha, \beta)$

$t_1, \dots, t_K$  known;  $\alpha$  known.

'Hyperprior'  $\beta \sim \text{Ga}(c, d)$ .  $c, d$  known.

Inference based on posterior distribution

$$\pi(\underline{\theta}, \beta | \underline{Y}) \propto \mathcal{L}(\underline{Y} | \underline{\theta}) \prod_{i=1}^K f_1(\theta_i | \beta) f_2(\beta)$$

$$= \left\{ \prod_{i=1}^K \frac{(\theta_i t_i)^{Y_i} e^{-\theta_i t_i}}{Y_i!} \right\} \times \left\{ \prod_{i=1}^K \frac{1}{\Gamma(\alpha) \beta^\alpha} \theta_i^{\alpha-1} e^{-\theta_i/\beta} \right\} \times \frac{1}{\Gamma(c) d^c} \beta^{c-1} e^{-\beta/d}$$

$$\propto \left\{ \prod_{i=1}^K (\theta_i t_i)^{Y_i} e^{-\sum_{i=1}^K \theta_i t_i} \right\} \frac{\text{constants} \prod_{i=1}^K \theta_i^{\alpha-1} e^{-\sum \theta_i/\beta}}{\beta^{c-1-K\alpha} e^{-\beta/d}}$$

Full condit. : ~~only keep~~

$$\pi(\theta_i | \beta, \underline{Y}) \propto (\theta_i t_i)^{Y_i} e^{-\theta_i t_i} \theta_i^{\alpha-1} e^{-\theta_i/\beta}$$

$$\propto \theta_i^{Y_i + \alpha - 1} e^{-\theta_i(t_i + 1/\beta)} \propto \text{Gamma}(Y_i + \alpha, t_i + 1/\beta)$$

$$= \theta_i^{(Y_i + \alpha) - 1} e^{-\theta_i / (t_i + 1/\beta)^{-1}} \propto \text{Gamma}(Y_i + \alpha, (t_i + 1/\beta)^{-1})$$

Recognized density! Simulate from Gamma directly, a Gibbs' update (posterior)  
In fact ~~if~~ priors ~~that~~ result in same type of distr.  
for a given likelihood are called 'conjugate' priors.

Note: conjugate priors are ~~often~~ <sup>commonly</sup> used to make computation simpler but they should not be used without a good (non-computing) justification — M-H algorithm works even if full conditl. is not <sup>of</sup> recognizable form.

Above example: Gamma is conjugate prior for Poisson.

Other example: Normal prior for mean of normal ; Beta prior for Binomial probability ( $p$ ) etc.

$$\pi(\beta | \underline{\theta}, \underline{y}) \propto e^{-\sum_{i=1}^k \theta_i / \beta} \beta^{c-1-a} e^{-\beta/d} = h(\beta | \underline{\theta}, \underline{y}), \text{ say}$$

Not recognizable density.

M-H algorithm / update: e.g. simplest one

Propose  $\beta^* \sim N(\beta_{\text{current}}, \tau^2)$

Accept-reject via M-H prob. ↑  
tuning parameter

So an M-H algorithm for  $\pi(\underline{\theta}, \beta | \underline{y})$  is:

1) Start M.C. at  $(\underline{\theta}^{(1)}, \beta^{(1)})$  initial values  
any value that is reasonably likely under  $\pi$  is fine.

2) Nth update of each  $\theta_i$  for  $i=1, \dots, k$  is according to

$$\pi(\theta_i | \underbrace{\theta_1, \dots, \theta_{i-1}, \theta_{i+1}, \dots, \theta_k}_{\text{most recent values}}, \beta, \underline{y})$$

For this simple example above is just  $\pi(\theta_i | \beta, \underline{y})$   
 $= \text{Gamma}(y_i + a, [t_i + \frac{1}{\beta}]^{-1})$  by condit. indep.  
 of  $\theta_i$ 's given  $\beta$ .

Sample  $\theta_i^{(n)} \sim \text{Gamma}(y_i + a, (t_i + \frac{1}{\beta^{(n)}})^{-1})$  for  $i=1, \dots, k$ .

3) Nth update of  $\beta$  is according to  $\pi(\beta | \underline{\theta}, \underline{y})$ .  
 Gibbs' update: always accept

Propose  $\beta^* \sim N(\beta^{(n)}, \tau^2)$

Accept w/ prob.  $\alpha(\beta, \beta^* | \underline{\theta}, \underline{y}) = \min \left\{ 1, \frac{h(\beta^* | \underline{\theta}, \underline{y}) q(\beta | \beta^*)}{h(\beta^{(n)} | \underline{\theta}, \underline{y}) q(\beta^* | \beta)} \right\}$

4) Return to step (2).

M.C. produced has stationary distr.  $\pi(\underline{\theta}, \beta | \underline{y})$  and  
 is Harris ergodic

Some other options:

⇒ depend on current value of  $\beta$

① Propose  $\beta^* \sim \text{Gamma}(\gamma_1(\beta), \gamma_2(\beta))$

w/ <sup>mean</sup>  $\gamma_1$  = current value and variance  $\gamma_2$

$$\text{so, } \gamma_1(\beta) \gamma_2(\beta) = \beta \quad \text{and} \quad \gamma_1(\beta) \gamma_2(\beta) = \gamma^2$$

$$\Rightarrow \gamma_2(\beta) = \gamma^2 / \beta \quad \text{and} \quad \gamma_1(\beta) = \beta / \gamma_2(\beta) = \beta^2 / \gamma^2$$

$q(\beta, \beta^*) \neq q(\beta^*, \beta)$  so M-H accept prob.

$$= \alpha(\beta, \beta^*) = \min \left\{ 1, \frac{h(\beta^* | \underline{\theta}, \underline{y})}{h(\beta | \underline{\theta}, \underline{y})} \frac{q(\beta, \beta^*)}{q(\beta^*, \beta)} \right\}$$

where  $q(\beta, \beta^*) = \text{Gamma}(\gamma_1(\beta), \gamma_2(\beta))$  pdf evaluated at  $\beta^*$ .

② ~~Log~~ Log-transform  $\beta$ , i.e., set  $\psi = \log \beta \in (-\infty, \infty)$   
Now use random-walk M-H update to sample from  $\psi | \underline{\theta}, \underline{y}$ .

Can transform to get  $\beta$  draws, i.e.,  $\beta = \exp(\psi)$ .

③ Laplace approx. for  $\pi(\beta | \underline{\theta}^{(n)}, \underline{y})$  as proposal  $q(\beta, \beta^*)$ .

Some basic M.C. theory for discrete time,  
contns. state spaces. (Borrowing from Jones & Hobert, 2001)

M.C.:  $X_0, X_1, X_2, \dots$   $X_i \in \Omega$

Discrete state space: t.p.m.  $\{P_{ij}\}$  where  $P_{ij} = \Pr(\text{move to state } j \text{ from state } i) = P(X_n = j | X_{n-1} = i)$   $i, j \in \Omega$

Contns. state space: transition density (more generally, the 'transition kernel') is a condtd pdf,  $K(x, y) = k(y|x)$  s.t.

$$P(X_n \in A | X_{n-1} = x) = \int_A K(y|x) dy \quad \forall x \in \Omega, \text{ all intervals } A.$$

Technically:  $\forall x \in \Omega, \forall A \in \mathcal{B}(\Omega)$

Borel  $\sigma$ -algebra generated by  $\Omega$   
(collection of subsets of  $\Omega$ )

$K^n(x, y)$  is  $n$ -step transition kernel

$$P(X_{i+n} \in A | X_i = x) = \int_A K^n(y|x) dy$$

This is an M.C. so

$$\begin{aligned} P(X_n \in A | X_{n-1} = x_{n-1}, X_{n-2} = x_{n-2}, \dots) &= P(X_n \in A | X_{n-1} = x_{n-1}) \\ &= \int_A K(y|x_{n-1}) dy \end{aligned}$$

E.g. of M.C. on continu. state space: AR(1) model

$$X_n = \theta X_{n-1} + \varepsilon_n \quad \theta \in \mathbb{R}$$

$$\varepsilon_1, \varepsilon_2, \dots \stackrel{\text{i.i.d.}}{\sim} N(0, \sigma^2)$$

$$P(X_n \in A | X_{n-1} = x_{n-1}, X_n = x_n, \dots)$$

$$= P(X_n \in A | X_{n-1} = x_{n-1}) = \int f(x_n = x | x_{n-1}) dx$$

where  $f(x_n | x_{n-1}) = \text{pdf of } \overset{A}{\text{~~the distribution~~}} N(\theta x_{n-1}, \sigma^2)$

Stationarity: if  $\pi$  is a density s.t.

$$\pi(y) = \int K(y|x) \pi(x) dx$$

then  $\pi$  is the stationary density for the M.C. defined by  $K$ .

If the current state of the chain is drawn from  $\pi$ , then marginal density of next state is also  $\pi$ . (Analogous to discrete state space M.C.'s).



## Irreducibility

M.C. can reach all interesting (positive prob.) regions (sets/intervals) in the state space.

Discrete case:  $\forall i, j \in \Omega, \exists n$  s.t.  $P_{ij}^n > 0$ .

Continuous state space:  $\pi$ -irreducibility

Let  $\pi(A) = \int_A \pi(x) dx$  (slight abuse of notation  $\pi$ )

M.C. is  $\pi$ -irreducible if  $\forall x \in \Omega$  and all  $A$  s.t.  $\pi(A) > 0$ ,  $\exists n$  s.t.  $P^n(x, A) > 0$ .

That is, any set w/ positive prob. under  $\pi$  is accessible from every pt. in state space.

## Recurrence

Discrete M.C.:  $\forall i \in \Omega$ ,  $P(X_n = i | X_0 = i) = 1$  for some  $n < \infty$ .

M.C. will return to state  $i$  after leaving state  $i$ , in a finite # of steps w/ prob. 1.

Equivalently all states will be visited infinitely often by M.C.

More general state spaces:

All interesting states will be visited infinitely often from 'almost-all' starting values.

A  $\pi$ -irreducible M.C. is recurrent if for all

$A$  s.t.  $\pi(A) > 0$ :

- (1)  $P(X_n \in A \text{ infinitely often} | X_0 = x) > 0 \quad \forall x \in \Omega$  and
- (2)  $P(X_n \in A \text{ infinitely often} | X_0 = x) = 1$  for  $\pi$ -almost all  $x$ , i.e.  $\forall x \in \Omega$  except possibly on a set  $N$  s.t.  $\pi(N) = 0$ .

$\pi$ -irreducible M.C. is positive recurrent if  $\pi$  is a prob. distr.

Allowing for a set of starting values from where we may not reach all  $A$  infinitely often is a nuisance

Positive Harris recurrence: A  $\pi$ -irreducible M.C. is positive Harris recurrent if for all  $A$  with  $\pi(A) > 0$ ,  $P(X_n \in A \text{ infinitely often} | X_0 = x) = 1 \forall x \in \Omega$ , and  $\pi$  is a prob. distr.

E.g. of pos-recurrent but non-Harris chain (Roberts & Rosenthal).

Aperiodicity:

Discrete case: Recall that period of state  $i$ ,  $d(i)$ , is gcd of all  $n \geq 1$  s.t.  $P_{ii}^n > 0$ .

If M.C. is aperiodic  $d(i) = 1 \forall i \in \Omega$

General case (g.c.tus) case: definition is more technical

Intuition: An M.C. is aperiodic if we cannot partition  $\Omega$  s.t. M.C. makes a regular tour through partition.

Regular tour would mean it only visits certain blocks at certain ~~intervals~~ times, say  $n = 2, 4, 6, 8, \dots$

Markov chains for MCMC.

If M.C. satisfies the following regularity conditions ('well behaved' for MCMC):

- (1) Aperiodicity      (2) Positive Harris recurrence.  
then M.C. is Harris-ergodic.

Thm. 1: If an M.C.  $(X_1, X_2, \dots)$  has stationary distr.  $\pi$  and is Harris-ergodic, SLLN holds:

If  $\mu = E\pi(g(X)) < \infty$  then

$$\hat{\mu}_n = \frac{\sum_{i=1}^n g(X_i)}{n} \rightarrow \mu \quad \text{w/ prob. 1.}$$

Note (1) This looks exactly like iid M. Carlo case except before:  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \pi$   
now:  $X_1, \dots, X_n$  are dependent and  $X_i$ 's are not distr. according to  $\pi$ .

$E(\hat{\mu}_n) \neq \mu$  unless M.C. is stationary,

so  $\hat{\mu}_n$  is usually a biased estimate of  $\mu$ .

- (2) Not easy to estimate  $\text{Var}(\hat{\mu}_n)$  and C.L.T. may not hold even if  $\text{Var}_{\pi}(g(X)) < \infty$   
MCMC !!

③ Although estimate is biased unless  $X_1 \sim \pi$ ,  
SLLN holds regardless of initial value distribution.

M-H algorithm lets us construct an <sup>Markov-ergodic</sup> M.C.  $\pi$  w/  
stationary distr.  $\pi$ , so SLLN ~~satisfied~~ holds.