

# MARKOV CHAIN MONTE CARLO:

Def: a collection  $\{m_i\}$  is called a Markov chain if the distribution of  $m_k$  depends **ONLY** on the immediate previous state  $m_{k-1}$  (tomorrow depends on the past only through today).

Def: We call the probability of  $m_k$  inside a set  $A$  starting from  $m_{k-1}$  as the transition probability:  $\mathbb{P}(m_{k-1}, A)$ . Abuse of notation:

$$\mathbb{P}(m_{k-1}, A) \stackrel{\text{def}}{=} \int_A \underbrace{\mathbb{P}(m_{k-1}, m)}_{\text{density}} dm$$

$$\stackrel{\text{def}}{=} \int_A \mathbb{P}(m_{k-1}, dm)$$

Notice:  $0 \leq \mathbb{P}(m_{k-1}, A) \leq 1$

$$\mathbb{P}(m_{k-1}, S) = \int_S \mathbb{P}(m_{k-1}, m) dm = 1$$

Example: Define transition matrix

$$P = \begin{pmatrix} 1/2 & 1/2 & 0 & 0 & \dots \\ 0 & 1/2 & 1/2 & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix}$$

Example: Regime Transition Matrix

$$P = \begin{bmatrix} 0 & 1/2 & 0 & 1/2 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2 & 1/2 \\ 1/3 & 1/3 & 0 & 0 & 1/3 \\ 0 & 0 & 1/2 & 1/2 & 0 \end{bmatrix}$$

$j$ th row is the transition probability to all nodes starting from node  $j$

Let  $m_{k-1} = L_1$ , Then the probability kernel (or density)  $\mathbb{P}[m_{k-1} = L_1, m]$

$$\mathbb{P}[m_{k-1} = L_1, m] = \mathbb{P}(L_1, :) = \left[ \frac{1}{3}, \frac{1}{3}, 0, 0, \frac{1}{3} \right]$$

$$\parallel$$

$$[0, 0, 0, 1, 0] \times P$$

Observation:  $\mathbb{P}[m_{k-1}, m_k]$  is the joint density between  $m_{k-1}, m_k$ .

$$\mathbb{P}[m_{k-1} = L_1, m_k = \cdot]$$

$$\parallel A = \{1\}$$

$$\int \mathbb{P}[m_{k-1} = L_1, m] dm$$

$$A = \{1\} \quad || \quad \mathbb{1}_A(x) = \begin{cases} 1 & x \in A \\ 0 & \text{otherwise} \end{cases}$$

$$\int_S P(m_{k-1} = 1, m) \mathbb{1}_A(m) dm$$

|| discrete case

$$\sum_{j=1}^5 P(m_{k-1} = 1, m) \delta(m-1)$$

$$= P(1, 1) = 1/3$$

Def : (Invariant distribution)

we say  $\mu(dm) = \pi(m) dm$  is an invariant distribution of the transition probability  $P(m_k, dm)$  if

$$\mu(dm) = \pi(m) dm = \int_S P(m_k, dm) \pi(m_k) dm_k$$

|| linear operator

$$\langle P(m_k, dm), \pi(m_k) dm_k \rangle$$

side note

Def : (Reversibility = detailed balance)

A Markov chain  $\{m_i\}$  is reversible w.r.t.  $\pi(m)$  if

$$\pi(m) P(m, p) = \pi(p) P(p, m)$$

$$\forall m, p \in \{m_i\}$$

Proof: 
$$\int_S \pi(m) P(m, p) dm = \int_S \pi(p) P(p, m) dm$$

$$= \pi(p) \int_S P(p, m) dm = \pi(p)$$

$\Rightarrow$  if  $\{m_i\}$  is reversible w.r.t.  $\pi(m)$   
 $\Rightarrow \pi(m)$  is an invariant distribution of  $\{m_i\}$ .

- Reversibility, roughly speaking, means that the likelihood of moving from  $m \rightarrow p$  is the same as the likelihood of moving from  $p \rightarrow m$ .

Proposition: if  $\{m_i\}$  is reversible w.r.t.  $\pi(m)$

then  $\pi(m)$  is an invariant distribution

$$\pi(m) dm = \int P(p, m) \pi(p) dp dm$$

$$\pi(m) dm = \int \underline{p}(p, m) \pi(p) dp dm$$


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## Markov chain Monte Carlo (MCMC)

- In general it is hard, if not impossible, to generate i.i.d. samples from  $\pi(m)$
- MCMC method is a universal approach to generate NON i.i.d. samples from  $\pi(m)$  while still preserving the LLN-like result.
- MCMC methods generates reversible (w.r.t.  $\pi$ ) Markov chain

Algorithm: Metropolis - Hastings MCMC method.

Choose initial state  $m_0$

For  $k = 0, \dots$  do

- 1) Draw a sample  $p$  from a Given/  
chosen proposal density  $q(m_k, p)$
- 2) Compute  $\pi(p), \pi(m_k)$   
 $q(m_k, p), q(p, m_k)$

3) Compute the acceptance probability  
(Metropolization)

$$\alpha(m_k, p) = \min \left\{ 1, \frac{\pi(p) q(p, m_k)}{\pi(m_k) q(m_k, p)} \right\}$$

4) \* accept  $p$  with probability  $\alpha(m_k, p)$   
    set  $m_{k+1} = p$   
    \* otherwise reject  $p$ : set  $m_{k+1} = m_k$

Question: is  $\pi(m)$  an invariant distribution  
of  $\{m_0, m_1, \dots\}$

— we have seen that if the reversibility holds  
then  $\pi(m)$  is an invariant distribution.

What remains is to show that MCMC algorithm  
generate transition probability that satisfies the  
detailed balance equation

Prop: the Markov chain generated from the  
above algorithm is reversible w.r.t  $\pi(m)$ .

Proof: we need to identify  $P(m_k, m_{k+1})$  and then

show 
$$\pi(m_k) P(m_k, m_{k+1}) \stackrel{??}{=} \pi(m_{k+1}) P(m_{k+1}, m_k)$$

Two cases:

1) Assume  $p$  is accepted:  $m_{k+1} = m_k$

2)  $p$  is rejected:  $m_{k+1} = m_k$

Let's work with the first case:  $P(m_k, m_{k+1})$  is joint probability of  $m_k, m_{k+1} = p$  where  $p = m_{k+1}$  is drawn from  $q(m_k, p)$  and  $p = m_{k+1}$  is accepted.

- define  $B$  as the acceptance event:

$$P(m_k, p) = \pi(B, p) \\ = \pi(B | p) \pi(p)$$

$$\begin{aligned} \parallel \quad \pi(p) &= q(m_k, p) \\ \parallel \quad \pi(B | p) &= \alpha(m_k, p) \end{aligned}$$

$$\alpha(m_k, p) q(m_k, p)$$

Question:  $\pi(m_k) P(m_k, p) \stackrel{??}{=} \pi(p) P(p, m_k)$

$$\left. \begin{aligned} &\pi(m_k) q(m_k, p) \min \left\{ 1, \frac{\pi(p) q(p, m_k)}{\pi(m_k) q(m_k, p)} \right\} \\ &\parallel \quad \pi(p) q(p, m_k) \min \left\{ 1, \frac{\pi(m_k) q(m_k, p)}{\pi(p) q(p, m_k)} \right\} \end{aligned} \right\}$$

we have  $\pi(m_k) P(m_k, p)$

$$\| \quad \underline{P}(m_k, p) = \alpha(m_k, p) q(m_k, p) \\ \pi(m_k) \propto(m_k, p) q(m_k, p)$$

$$\| \text{def } \alpha$$

$$\frac{\pi(m_k) q(m_k, p)}{\pi(p) q(p, m_k)} \min \left\{ 1, \frac{\pi(p) q(p, m_k)}{\pi(m_k) q(m_k, p)} \right\} \\ a \min \{c, d\} \quad \| = \min \{ac, ad\}$$

$$\min \left\{ \pi(m_k) q(m_k, p), \pi(p) q(p, m_k) \right\}$$

$$\| \min \{ac, ad\} = a \min \{c, d\}$$

$$\min \left\{ \frac{\pi(m_k) q(m_k, p)}{\pi(p) q(p, m_k)}, 1 \right\} \pi(p) q(p, m_k)$$

$$\| \text{def } \alpha$$

$$\alpha(p, m_k) \pi(p) q(p, m_k)$$

$$\| \text{def transition probability } \underline{P}(\cdot, \cdot)$$

$$\pi(p) \underline{P}(p, m_k)$$

$\Rightarrow$  the resulting Markov chain is reversible



w.r.t  $\pi(m)$



$\pi(m)$  is ~~AN~~ invariant measure for  $\{m_i\}$

??  $\Downarrow$  understood

$\{m_i\}$  is eventually distributed by  $\pi(m)$

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Is  $\{m_i\}$  distributed by  $\pi(m)$ ?

Def: (Irreducibility). If

1)  $\pi(m)$  is finite everywhere.

2)  $q(\cdot, \cdot)$  is positive and continuous

then  $\{m_i\}$  is