# Lecture 10:

# Reversibility; the Metropolis-Hastings Algorithm

## Part I: Reversibility

Let $P$ be a transition matrix with a stationary distribution $\vec{\pi}$. Let $(X_n)_{n\geq 0}$ be a realization of this Markov chain starting from the stationary distribution, i.e., $X_0 \sim \vec{\pi}$. ($\mathbb{P}(X_0 = i) = \vec{\pi}_i$, $\forall i \in \mathcal{X}$).

Fix $n \in \mathbb{N}$. Let $Y_m := X_{n-m}$ for $0 \leq m \leq n$, which is called the time reversal of the process $\{X_m\}_{0\leq m\leq n}$.

Q: Is $\{Y_m\}_{0\leq m\leq n}$ a Markov chain? why?

A: Let us compare $\mathbb{P}(Y_{m+1} = i_{m+1} \mid (Y_k)_{0\leq k\leq m} = (i_k)_{0\leq k\leq m})$ with $\mathbb{P}(Y_{m+1} = i_{m+1} \mid Y_m = i_m)$.

$$\mathbb{P}(Y_{m+1} = i_{m+1} \mid Y_m = i_m, \cdots, Y_0 = i_0)$$

$$= \frac{\mathbb{P}(Y_{m+1} = i_{m+1}, Y_m = i_m, \cdots, Y_0 = i_0)}{\mathbb{P}(Y_m = i_m, Y_{m-1} = i_{m-1}, \cdots, Y_0 = i_0)}$$

$$= \frac{\mathbb{P}(X_n = i_0, X_{n-1} = i_1, \cdots, X_{n-m} = i_m, X_{n-m-1} = i_{m+1})}{\mathbb{P}(X_n = i_0, X_{n-1} = i_1, \cdots, X_{n-m} = i_m)}$$

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$$= \frac{\mathbb{P}(X_n = i_0, \cdots, X_{n-m+1} = i_{m-1} \mid X_{n-m} = i_m) \cdot \mathbb{P}(X_{n-m} = i_m, X_{n-m-1} = i_{m+1})}{\mathbb{P}(X_n = i_0, \cdots, X_{n-m+1} = i_{m-1} \mid X_{n-m} = i_m) \cdot \mathbb{P}(X_{n-m} = i_m)}$$

$$= \frac{\mathbb{P}(X_{n-m} = i_m \mid X_{n-m-1} = i_{m+1}) \cdot \mathbb{P}(X_{n-m-1} = i_{m+1})}{\mathbb{P}(X_{n-m} = i_m)}$$

$$= \frac{P_{i_{m+1} i_m} \cdot \vec{\pi}_{i_{m+1}}}{\vec{\pi}_{i_m}} .$$

On the other hand, $\mathbb{P}(Y_{m+1} = i_{m+1} \mid Y_m = i_m)$

$$= \frac{\mathbb{P}(Y_{m+1} = i_{m+1}, Y_m = i_m)}{\mathbb{P}(Y_m = i_m)}$$

$$= \frac{\mathbb{P}(X_{n-m} = i_m, X_{n-m-1} = i_{m+1})}{\mathbb{P}(X_{n-m} = i_m)} = \frac{P_{i_{m+1} i_m} \cdot \vec{\pi}_{i_{m+1}}}{\vec{\pi}_{i_m}} .$$

Thus, $\mathbb{P}(Y_{m+1} = i_{m+1} \mid (Y_k)_{0 \le k \le m} = (i_k)_{0 \le k \le m}) = \mathbb{P}(Y_{m+1} = i_{m+1} \mid Y_m = i_m)$

$$= \frac{P_{i_{m+1} i_m} \cdot \vec{\pi}_{i_{m+1}}}{\vec{\pi}_{i_m}} , \qquad \forall m \in [0, n-1], \forall (i_k)_{k \in [0, m+1]} \in \mathcal{X}^{m+2} .$$

Therefore, $\{Y_m\}_{m \in [0,n]}$ is a time homogeneous Markov chain with transition probability

$$\hat{P}_{xy} := \mathbb{P}(Y_{m+1} = y \mid Y_m = x) = \frac{P_{yx} \cdot \vec{\pi}_y}{\vec{\pi}_x} .$$

**Theorem 10.1.** Fix $n$, the time reversal of $\{X_m\}_{m\in[0,n]}$ is also a time homogeneous Markov chain with transition probability

$$\hat{P}_{xy} := \mathbb{P}(Y_{m+1}=y \mid Y_m = x) = \frac{P_{yx}\cdot \vec{\pi}_y}{\vec{\pi}_x},$$

this is also called the dual transition probability of $P$.

**Cor 9.1.** When $\vec{\pi}$ satisfies the detailed balance condition

$$\vec{\pi}_x P_{xy} = \vec{\pi}_y P_{yx}, \quad \forall x,y \in \mathcal{X},$$

then $\hat{P}$ satisfies

$$\hat{P}_{xy} = \frac{P_{yx}\cdot \vec{\pi}_y}{\vec{\pi}_x} = P_{xy}, \quad \forall x,y \in \mathcal{X},$$

and $\hat{\vec{\pi}}$ also satisfies the detailed balance condition

$$\hat{\vec{\pi}}_x \hat{P}_{xy} = \hat{\vec{\pi}}_y \hat{P}_{yx}, \quad \forall x,y \in \mathcal{X},$$

because $\hat{\vec{\pi}}_i = \vec{\pi}_i, \ \forall i \in \mathcal{X}$.

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Part II.

Goal: Generating samples from given probability density $\vec{\pi}$.

Strategy: Build a Markov chain with $\vec{\pi}$ being its stationary distribution.

Start: Begin with a Markov chain with transition matrix $Q$.

Check: If $\vec{\pi}$ satisfies the detailed balance condition with $Q$, i.e., $\vec{\pi}_x Q_{xy} = \vec{\pi}_y Q_{yx}$, $\forall x, y \in \mathcal{X}$, then $\vec{\pi}$ is a stationary distribution of this Markov chain which we can sample from. If not, revise $Q$.

Revision: Starting from any state $x$, a move to another state $y$ is accepted with probability

$$R_{xy} = \min \left\{ \frac{\vec{\pi}_y Q_{yx}}{\vec{\pi}_x Q_{xy}}, 1 \right\}.$$

So the chain follows a new transition probability

$$P_{xy} = \begin{cases} Q_{xy} \cdot R_{xy}, & y \neq x. \\ 1 - \sum_{y \neq x} Q_{xy} R_{xy}, & y = x. \end{cases}$$

**Theorem 10.2.** Under the above algorithm, $\vec{\pi}$ satisfies the detailed balance condition with the new transition matrix $P$, i.e., $\vec{\pi}_x P_{xy} = \vec{\pi}_y P_{yx}$, $\forall\, x, y \in \mathcal{X}$.

Thus $\vec{\pi}$ is a stationary distribution of this chain.

Pf. ① If $x$ and $y$ satisfies $\vec{\pi}_x Q_{xy} = \vec{\pi}_y Q_{yx}$, then

$$R_{xy} = R_{yx} = 1, \quad P_{xy} = Q_{yx}, \quad P_{yx} = Q_{yx}.$$

Thus, $\vec{\pi}_x P_{xy} = \vec{\pi}_x Q_{xy} = \vec{\pi}_y Q_{yx} = \vec{\pi}_y P_{yx}$.

② If $\vec{\pi}_x Q_{xy} > \vec{\pi}_y Q_{yx}$, then

$$R_{xy} = \frac{\vec{\pi}_y Q_{yx}}{\vec{\pi}_x Q_{xy}}, \quad R_{yx} = 1,$$

and $P_{xy} = Q_{xy} R_{xy} = \dfrac{\vec{\pi}_y Q_{yx}}{\vec{\pi}_x}$, $P_{yx} = Q_{yx} R_{yx} = Q_{yx}$.

This implies, $\vec{\pi}_x \cdot P_{xy} = \vec{\pi}_y Q_{yx} = \vec{\pi}_y \cdot P_{yx}$.

③. If $\vec{\pi}_x Q_{xy} < \vec{\pi}_y Q_{yx}$, then similar to ②, we also have

$\vec{\pi}_x \cdot P_{xy} = \vec{\pi}_y \cdot P_{yx}$.

Therefore, $\vec{\pi}$ satisfies the detailed balance condition with $P$,

$$\vec{\pi}_x \cdot P_{xy} = \vec{\pi}_y \cdot P_{yx}, \quad \forall x, y \in \mathcal{X}. \qquad \blacksquare$$

Remark 10.1. To generate one sample from $\vec{\pi}$, we run the chain for a long time so that it reaches equilibrium. To obtain many samples, we output the states at widely separated times (, so that these output are not correlated). If we are interested in the expected value of a function on the state space $f: \mathcal{X} \to \mathbb{R}$, suppose the chain is irreducible and $\mathcal{X}$ is finite, we can calculate $\mathbb{E}_\pi f = \sum_{x \in \mathcal{X}} f(x) \vec{\pi}_x$ as a limit of $\frac{1}{n} \sum_{k=0}^{n-1} f(X_k)$, which is guaranteed by Theorem 9.4.

**Ex 1.** (Geometric distribution) Let $0<\theta<1$ and $\pi_x = \theta^x(1-\theta)$, $\forall x \in \mathbb{N}$.

Let $Q_{x,x-1} = Q_{x,x+1} = \frac{1}{2}$, $\forall x \geq 1$; and $Q_{01} = Q_{00} = \frac{1}{2}$.

Then $R_{xy} = \min\left\{ \frac{\pi_y Q_{yx}}{\pi_x Q_{xy}}, 1 \right\} = \min\left\{ \frac{\pi_y}{\pi_x}, 1 \right\}$.

① If $x>0$, one has $\pi_{x-1} > \pi_x > \pi_{x+1} = \theta \pi_x$.

Thus $P_{x,x-1} = \frac{1}{2}$, $P_{x,x+1} = \frac{\theta}{2}$, $P_{x,x} = 1 - \frac{1}{2} - \frac{\theta}{2} = \frac{1}{2} - \frac{\theta}{2}$,

and $P_{xy} = 0$, $\forall |y-x| > 1$.

② If $x=0$, then $P_{0,1} = \frac{\theta}{2}$, $P_{0,0} = 1 - \frac{\theta}{2}$, and

$P_{xy} = 0$, $\forall |y-x| > 1$.

Therefore, $\pi_x P_{x,x+1} = \theta^x(1-\theta) \cdot \frac{\theta}{2} = \pi_{x+1} \cdot P_{x+1,x}$, $\forall x \in \mathbb{N}$.

For $\theta$ close to 1, choose

$$Q_{x,x+i} = \frac{1}{2L+1}, \quad \forall -L \leq i \leq L,$$

where $L = O\left(\frac{1}{1-\theta}\right)$ to make the chain move around the state space faster while not having two many steps rejected.

*This is the end of this lecture!*