

Markov Chain Monte Carlo
Theory and Practical applications
Chapters 2 and 3

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Outline

- ① Chap 2: Some recaps
- ② Chap 2: Uniqueness of invariant probability measures
- ③ Chap 3: Dynamical systems
- ④ Chap 3: Markov chains and ergodicity

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- 2 Chap 2: Uniqueness of invariant probability measures
- 3 Chap 3: Dynamical systems
- 4 Chap 3: Markov chains and ergodicity

Recall that a Markov kernel P is

- 1 π -invariant if $\pi P = \pi$
- 2 π -reversible if $\pi(dx)P(x, dy) = \pi(dy)P(y, dx)$
- 3 π -reversible implies π -invariance.

The Metropolis-Hastings algorithm

Input: n

Output: X_0, \dots, X_n

- At $t = 0$, draw X_0 according to some arbitrary distribution
- For $t \leftarrow 0$ to $n - 1$
 - 1 Draw independently $Y_{t+1} \sim \mathbf{Q}(X_t, \cdot)$ and $U_{t+1} \sim \text{Unif}(0, 1)$
 - 2 Set $X_{t+1} = \begin{cases} Y_{t+1} & \text{if } U_{t+1} \leq \alpha(X_t, Y_{t+1}) \\ X_t & \text{otherwise} \end{cases}$

where $\alpha(x, y) = \alpha^{MH}(x, y) = \min\left(\frac{\pi(y)q(y, x)}{\pi(x)q(x, y)}, 1\right)$

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The Markov kernel associated to $\{X_n : n \in \mathbb{N}\}$ is given by

$$P_{\langle \pi, Q \rangle}^{MH}(x, dy) = Q(x, dy)\alpha(x, y) + \bar{\alpha}(x)\delta_x(dy).$$

where $\bar{\alpha}(x) = 1 - \int_{\mathcal{X}} Q(x, dy)\alpha(x, y)$.

Lemma

If the detailed balance condition

$$\pi(dx)Q(x, dy)\alpha(x, y) = \pi(dy)Q(y, dx)\alpha(y, x) \quad (1)$$

is satisfied, then $P_{\langle \pi, Q \rangle}^{MH}$ is π -reversible and hence, π -invariant.

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- For all α satisfying (1), we have $\alpha \leq \alpha^{MH}$. To be done on the blackboard.

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Uniqueness under irreducibility assumptions

Proposition: Irreducible Markov kernels

Assume that there exists a non-null measure $\mu \in M_+(\mathbf{X})$ satisfying the following property:

- ★ For all $A \in \mathcal{X}$ such that $\mu(A) > 0$ and for all $x \in \mathbf{X}$, there exists $n \in \mathbb{N}$ such that $P^n(x, A) > 0$.

Then, P admits **at most one** invariant probability measure.

If condition (★) is satisfied, we say that P is μ -irreducible.

Application: Metropolis-Hastings algorithms

Assume that

- $Q(x, dy) = q(x, y)\lambda(dy)$ and $\pi(dx) = \pi(x)\lambda(dx)$ with $q > 0$ and $\pi > 0$.

Then $P_{\langle \pi, Q \rangle}^{MH}$ admits π as its **unique probability measure**.

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Proof of the uniqueness of the invariant probability measure for irreducible Markov chains

The following lemma is useful for the proof...

Lemma

If P admits two distinct invariant probability measures, it also admits distinct invariant probability measures π_0 and π_1 that are mutually singular, i.e., such that there exists $A \in \mathcal{X}$ such that $\pi_0(A) = \pi_1(A^c) = 0$.

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Dynamical systems

Definition

(Dynamical systems) A dynamical system \mathcal{D} is a quadruplet $\mathcal{D} = (\Omega, \mathcal{F}, \mathbb{P}, T)$ where $(\Omega, \mathcal{F}, \mathbb{P})$ is a probability space and $T : \Omega \rightarrow \Omega$ is a measurable mapping such that $\mathbb{P} = \mathbb{P} \circ T^{-1}$.

Lemma

(Invariant sets) *The collection of sets $\mathcal{I} = \{A \in \mathcal{F} : \mathbf{1}_A = \mathbf{1}_A \circ T\}$ is a σ -field and any set in \mathcal{I} is called an invariant set.*

Definition

(Ergodicity) A dynamical system $(\Omega, \mathcal{F}, \mathbb{P}, T)$ is said to be ergodic if invariant sets are \mathbb{P} -trivial that is if $A \in \mathcal{I}$ then either $\mathbb{P}(A) = 0$ or $\mathbb{P}(A) = 1$.

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The Birkhoff theorem

Theorem

(The Birkhoff theorem) Let $\mathcal{D} = (\Omega, \mathcal{F}, \mathbb{P}, T)$ be an ergodic dynamical system and let $h \in L_1(\Omega)$. Then,

$$\lim_{n \rightarrow \infty} n^{-1} \sum_{k=0}^{n-1} h \circ T^k = \mathbb{E}[h], \quad \mathbb{P} - a.s.$$

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Let S be the shift operator: if $\omega = (\omega_k)_{k \in \mathbb{N}} \in \mathcal{X}^{\mathbb{N}}$, we set $S(\omega) = \omega' \in \mathcal{X}^{\mathbb{N}}$ where $\omega'_k = \omega_{k+1}$ for all $k \in \mathbb{N}$.

Lemma (MC and dynamical systems)

Let P be a Markov kernel admitting an *invariant probability measure* π . Then, the quadruplet $(\mathcal{X}^{\mathbb{N}}, \mathcal{X}^{\otimes \mathbb{N}}, \mathbb{P}_\pi, S)$ is a *dynamical system*.

Theorem (MC and ergodicity)

Let P be a Markov kernel on $X \times \mathcal{X}$. Assume that P admits a *unique invariant probability measure* π . Then, the dynamical system $(\mathcal{X}^{\mathbb{N}}, \mathcal{X}^{\otimes \mathbb{N}}, \mathbb{P}_\pi, S)$ is *ergodic*.

The proof of the Theorem will be done on the blackboard.

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Theorem (The Birkhoff theorem for MC)

Let P be a Markov kernel admitting a *unique invariant probability measure* π . Then, for all $h \in \mathcal{F}(X^{\mathbb{N}})$ such that $\mathbb{E}_{\pi}[|h|] < \infty$, we have

$$\lim_{n \rightarrow \infty} n^{-1} \sum_{k=0}^{n-1} h(X_{k:\infty}) = \mathbb{E}_{\pi}[h], \quad \mathbb{P}_{\pi} - a.s.$$

Corollary (LLN Starting from stationarity)

Let P be a Markov kernel admitting a *unique invariant probability measure* π . Then, for all $f \in \mathcal{F}(X)$ such that $\pi(|f|) = \int_X \pi(dx) |f(x)| < \infty$, we have

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Corollary (Other starting points)

Let P be a Markov kernel admitting a *unique invariant probability measure* π . Then, for all $f \in F(X)$ such that $\pi(|f|) = \int_X \pi(dx) |f(x)| < \infty$, we have **for π -almost all $x \in X$** ,

$$\lim_{n \rightarrow \infty} n^{-1} \sum_{k=0}^{n-1} f(X_k) = \pi(f), \quad \mathbb{P}_x - a.s. \quad (3)$$

Assume that $Q(x, dy) = q(x, y)\lambda(dy)$ and $\pi(dy) = \pi(y)\lambda(dy)$ where $q > 0$, $\pi > 0$ and λ is a σ -finite measure on (X, \mathcal{X}) .

Theorem

The Markov chain $\{X_n : n \in \mathbb{N}\}$ generated by the Metropolis-Hastings algorithm is such that: *for all initial distributions $\nu \in \mathbf{M}_1(X)$ and all $f \in F(X)$ such that $\int_X \pi(dx)|f(x)| < \infty$,*

$$\lim_{n \rightarrow \infty} n^{-1} \sum_{k=0}^{n-1} f(X_k) = \pi(f), \quad \mathbb{P}_\nu - a.s \quad (4)$$

What if P is not the Markov kernel of a Metropolis-Hastings algorithm?

Theorem

If P is a Markov kernel on $X \times \mathcal{X}$ that admits a **unique invariant probability measure** π . Assume in addition that for all bounded functions h and all measures $\nu \in M_1(X)$,

$$\lim_{n \rightarrow \infty} \nu P^n h = \pi(h) \quad (5)$$

Then, **for all initial distributions** $\nu \in M_1(X)$ and all $f \in F(X)$ such that $\pi(|f|) = \int_X \pi(dx) |f(x)| < \infty$,

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