

# Markov Chain Monte Carlo Methods

---

Juan F. Rubio-Ramírez

Emory University

“Bayesianism has obviously come a long way. It used to be that you could tell a Bayesian by his tendency to hold meetings in isolated parts of Spain and his obsession with coherence, self-interrogations, and other manifestations of paranoia. Things have changed...”

Peter Clifford (1993)

- We have a distribution:

$$X \sim f(X)$$

such that  $f > 0$  and  $\int f(x) dx < \infty$ .

- How do we draw from it?
- We could use Importance Sampling...
- ...but we need to find a good source density.

- The function  $P(x, A)$  is a transition kernel for  $x \in \mathcal{X}$  and  $A \in \mathcal{B}(\mathcal{X})$  (a Borel  $\sigma$ -field) such that:
  1. For all  $x$ ,  $P(x, \cdot)$  is a probability measure.
  2. For all  $A$ ,  $P(\cdot, A)$  is measurable.
- When  $\mathcal{X}$  is discrete,  $P_{xy} = P(X_n = y \mid X_{n-1} = x)$ .
- When  $\mathcal{X}$  is continuous,

$$P(X \in A \mid x) = \int_A P(x, x') dx'.$$

- Clearly  $P(x, \mathcal{X}) = 1$ .
- It may be that  $P(x, \{x\}) \neq 0$ .
- Examples in economics: capital accumulation, job search, prices in financial markets, ...

## A Particular Transition Kernel

Define:

$$P(x, dy) = p(x, y) dy + r(x) \delta_{\{x\}}(dy)$$

or

$$P(x, A) = \int_A p(x, y) dy + r(x) \int_A \delta_{\{x\}}(dy) = \int_A p(x, y) dy + r(x) 1_A(x)$$

1.  $p(x, y) \geq 0$ ,  $p(x, x) = 0$ .
2.  $\delta_{\{x\}}(dy)$  is the Dirac delta.
3.  $P(x, x)$ , the probability the chain stays at  $x$ , is  $r(x)$ .
4. By construction:

$$r(x) = 1 - \int_{\mathcal{X}} p(x, y) dy.$$

- Given a transition kernel  $P$ , a sequence  $X_0, X_1, \dots$  is a Markov Chain if for any  $k$

$$P(X_{k+1} \in A \mid x_0, \dots, x_k) = P(X_{k+1} \in A \mid x_k) = \int_A P(x_k, dx).$$

- We focus on **time-homogeneous** chains: the distribution of  $(X_{t_1}, \dots, X_{t_k})$  given  $x_{t_0}$  is the same as that of  $(X_{t_1-t_0}, \dots, X_{t_k-t_0})$  given  $x_0$ .

# Chapman–Kolmogorov Equations

- For a time-homogeneous chain:

$$P^{m+n}(x, A) = \int_{\mathcal{X}} P^n(y, A) P^m(x, dy).$$

- Implies convolution formula:  $P^{m+n} = P^m \star P^n$ .
- Discrete case: this is a matrix product. Continuous case:  $P$  acts as an operator:

$$Ph(dy) = \int_{\mathcal{X}} P(x, dy) h(x) dx.$$



# Two Important Questions in Markov Chains

Knowing  $P(x, B)$ :

- Does there exist a fixed point  $\pi_s$  such that

$$\pi_s(B) = \int_{\mathcal{X}} P(x, B) \pi_s(dx)?$$

- If  $P^1(x, dy) = P(x, dy)$ , does  $P^n(x, B) \rightarrow \pi_s(B)$  as  $n \rightarrow \infty$ ?
- Reference: Meyn & Tweedie (1993), *Markov Chains and Stochastic Stability*.

- Does there exist a kernel  $P(x, B)$  such that

$$\pi_s(B) = \int_{\mathcal{X}} P(x, B) \pi_s(dx)?$$

- If  $P^1(x, dy) = P(x, dy)$ , does  $P^n(x, B) \rightarrow \pi_s(B)$  as  $n \rightarrow \infty$ ?
- Reference: Chib & Greenberg (1995), “Understanding the Metropolis–Hastings Algorithm.”

- An MCMC method simulates  $f(x)$  by producing an ergodic Markov Chain with invariant distribution  $f(x)$ .
- We seek a chain such that if  $X^1, X^2, \dots, X^t$  are realizations,

$$X^t \rightarrow X \sim f(x)$$

as  $t \rightarrow \infty$ .

# Turning the Theory Around

- For equilibrium models: we know the kernel (policy functions)  $\rightarrow$  find invariant distribution.
- For MCMC: we know the invariant distribution  $\rightarrow$  find a kernel that produces it.
- Question: How do we find such a transition kernel?

We search for a transition kernel that:

1. Has stationary distribution  $f(x)$ .
2. Stays within that stationary distribution (convergence).
3. Converges to it.
4. Obeys a Law of Large Numbers.
5. Admits a Central Limit Theorem.

### Definition

The density  $f$  is stationary for a Markov kernel  $P$  if

$$\int_A f(y) dy = \int_{\mathcal{X}} f(x) P(x, A) dx \quad \forall A.$$

### Definition

The Markov kernel  $P$  is  $f$ -reversible if

$$\forall g \quad \iint g(x, y) f(x) dx P(x, dy) = \iint g(y, x) f(y) dy P(y, dx).$$

## Definition

The Markov kernel  $P$  is *time reversible* if

$$f(x) p(x, y) = f(y) p(y, x) \quad \text{for a.e. } (x, y).$$

where

$$P(x, dy) = p(x, y) dy + r(x) \delta_{\{x\}}(dy)$$

Then the following are equivalent:

- (i)  $P$  is  $f$ -reversible
- (ii)  $P$  is time reversible

**Proof.**

Expanding both sides of the  $f$ -reversibility condition, the singular terms involving  $\delta_x$  cancel automatically. The remaining absolutely continuous parts imply

$$\iint g(x, y) f(x) p(x, y) dx dy = \iint g(y, x) f(y) p(y, x) dy dx \quad \forall g,$$

which holds if and only if  $f(x)p(x, y) = f(y)p(y, x)$  a.e. □



Let  $f$  be a density and let  $P$  be a Markov kernel.

**Definition (Detailed balance)**

We say that  $(f, P)$  satisfies *detailed balance* if for all  $A, B$ ,

$$\int_B f(x) P(x, A) dx = \int_A f(y) P(y, B) dy.$$

## Lemma: Detailed Balance $\Rightarrow$ Stationary and Reversible

### Lemma

If  $(f, P)$  satisfies detailed balance, then

1.  $f$  is stationary for  $P$ , i.e. for all  $A$ ,

$$\int_{\mathcal{X}} f(x) P(x, A) dx = \int_A f(y) dy;$$

2.  $P$  is  $f$ -reversible, i.e. for all  $g$ ,

$$\iint g(x, y) f(x) dx P(x, dy) = \iint g(y, x) f(y) dy P(y, dx).$$

## Proof (Sketch)

### Proof sketch.

- **Stationarity:** Apply detailed balance with  $B = \mathcal{X}$ :

$$\int_{\mathcal{X}} f(x) P(x, A) dx = \int_A f(y) P(y, \mathcal{X}) dy = \int_A f(y) dy,$$

since  $P(y, \mathcal{X}) = 1$ .

- **$f$ -reversibility:** Detailed balance implies equality of the two measures,

$$\mu_1(dx, dy) := f(x) dx P(x, dy), \quad \mu_2(dx, dy) := f(y) dy P(y, dx),$$

because  $\mu_1(B \times A) = \mu_2(B \times A)$  for all measurable rectangles  $B \times A$ . Hence  $\mu_1 = \mu_2$ , and integrating any  $g$  yields the stated identity (we can use the monotone class theorem)

## Searching for a Transition Kernel $P(x, A)$

- Let  $P(x, dy) = p(x, y)dy + r(x)\delta_{\{x\}}(dy)$ .
- If  $f(x)p(x, y) = f(y)p(y, x)$  (time reversibility), then

$$\int_A f(y) dy = \int_{\mathcal{X}} P(x, A)f(x) dx.$$

- This means that  $f(x)$  is a stationary distribution.
- Time reversibility also called detailed balance.

$$\begin{aligned}\int_{\mathcal{X}} P(x, A) f(x) dx &= \int_{\mathcal{X}} \left[ \int_A p(x, y) dy \right] f(x) dx + \int_{\mathcal{X}} r(x) \delta_{\{x\}}(A) f(x) dx \\&= \int_A \left[ \int_{\mathcal{X}} p(x, y) f(x) dx \right] dy + \int_A r(x) f(x) dx \\&= \int_A \left[ \int_{\mathcal{X}} p(y, x) f(y) dx \right] dy + \int_A r(x) f(x) dx \\&= \int_A (1 - r(y)) f(y) dy + \int_A r(x) f(x) dx = \int_A f(y) dy.\end{aligned}$$

- The condition  $f(x)p(x, y) = f(y)p(y, x)$  ensures  $f$  is the invariant distribution.
- Time reversibility is the key property for MCMC algorithms.

- We proved  $f$  is a fixed point of the kernel operator.
- We ask: does  $P^m(x, A) \rightarrow \pi_s(A)$  as  $m \rightarrow \infty$ ?

# Sufficient Conditions for Convergence

If the kernel satisfies time reversibility and:

- **Irreducibility:** any  $x$  can reach any  $A$  with positive probability.
- **Aperiodicity:** chain does not have periodic behavior.
- A irreducible Markov chain is **Harris recurrent** if for any measurable set  $\mu(A) > 0$ , we have

$$\forall x \in \mathcal{X} \quad \mathbb{P}_x(\eta_A = \infty) = 1.$$

where

$$\eta_A = \sum_{k=1}^{\infty} 1_A(X_k)$$



# A Law of Large Numbers

If  $P(x, A)$  is irreducible and aperiodic with invariant distribution  $\pi_s$ :

1.  $\pi_s$  is unique.
2. For all integrable  $h$ :

$$\frac{1}{M} \sum_{i=1}^M h(x_i) \rightarrow \int h(x) \pi_s(dx),$$

i.e.

$$\hat{h} \rightarrow Eh.$$

We need a kernel  $P(x, A)$  such that:

1. Time reversible ( $f(x)$  invariant).
2. Irreducible (convergence + LLN).
3. Aperiodic (convergence + LLN).
4. Harris-recurrent and geometrically ergodic (CLT).

These are sufficient for validity of MCMC.

- The Metropolis–Hastings algorithm is the canonical MCMC method.
- Gibbs sampler is a special case.
- Many variants exist—be cautious!
- The frontier: Perfect Sampling.

- Motivation: draw from a posterior distribution.
- But MCMC applies more broadly:
  1. It can sample from any distribution, not necessarily Bayesian posteriors.
  2. It explores distributions and can be used for classical estimation as well.