Chapter 4

Markov Chain Monte Carlo.
Metropolis Algorithm.

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Markov Chains for Monte Carlo Estimation

We have been discussing inference using **Markov chains**.

- Concepts such as sampling and stationary distributions are central.
- For **discrete** Markov chains, dynamic programming algorithms can often be used for exact inference (e.g., Hidden Markov Models).

We can also use Markov chains for inference in more general settings.

- The most common framework is **Markov Chain Monte Carlo (MCMC)**.
- MCMC methods are used for **approximate inference**, particularly in complex Bayesian models (e.g., Bayesian logistic regression).

High-level idea of MCMC:

- We want to compute expectations with respect to a distribution $p(x)$, but we cannot generate independent samples directly from p.
- Construct a **homogeneous Markov chain** whose **stationary distribution** is $p(x)$.
- After a suitable burn-in period, use the generated samples $\{X_t\}_{t=1}^{T}$ in a Monte Carlo approximation.

Reminder: Homogeneous Markov Chains

Definition: A sequence of random variables $\{X_t\}_{t\geq 0}$ is a **Markov chain** if

$$P(X_{t+1} = j \mid X_t = i, X_{t-1}, \ldots, X_0) = P(X_{t+1} = j \mid X_t = i).$$

The process is called **homogeneous** (or time-homogeneous) if the transition probabilities do not depend on t:

$$P(X_{t+1} = j \mid X_t = i) = P_{ij}, \quad \text{for all } t.$$

Transition matrix:

$$\mathbf{P} = \begin{pmatrix} P_{11} & P_{12} & \cdots \\ P_{21} & P_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, \quad P_{ij} \geq 0, \quad \sum_j P_{ij} = 1.$$

n-step transition: $P^{(n)} = \mathbf{P}^n$, with entries $P_{ij}^{(n)} = P(X_{t+n} = j \mid X_t = i)$.

Stationary Distribution

Definition: A probability vector $\boldsymbol{\pi}$ is a **stationary distribution** of a Markov chain if

$$\boldsymbol{\pi}^\top \mathbf{P} = \boldsymbol{\pi}^\top, \quad \sum_i \pi_i = 1,\ \pi_i \geq 0.$$

Interpretation:If $X_0 \sim \boldsymbol{\pi}$ then $X_t \sim \boldsymbol{\pi}$ for all t. The chain remains in equilibrium under $\boldsymbol{\pi}$.

Convergence: For many Markov chains

$$\lim_{t\to\infty} P(X_t = j \mid X_0 = i) = \pi_j$$

Irreducibility, Recurrence, and Ergodicity

Irreducibility: A Markov chain is **irreducible** if every state can be reached from every other state:

$$\forall i, j,\ \exists n \text{ such that } P_{ij}^{(n)} > 0$$

Recurrence: State i is **recurrent** if, starting from i, the probability of returning to i is 1:

$$P(\text{return to } i \mid X_0 = i) = 1$$

If the expected return time is finite, i is **positive recurrent**.

Ergodicity: An irreducible, aperiodic (gcd is 1 for all possible return times to a state), and positive recurrent Markov chain is called **ergodic**. For ergodic chains,

$$\lim_{t \to \infty} P(X_t = j \mid X_0 = i) = \pi_j$$

and time averages converge to expectations under π:

$$\frac{1}{T} \sum_{t=1}^{T} f(X_t) \xrightarrow{a.s.} E_\pi[f(X)]$$

Degenerate Example: “Pointless MCMC”

Consider estimating the expected value of a fair six-sided die. We know analytically that

$$E[X] = \frac{1+2+3+4+5+6}{6} = 3.5$$

Now suppose we design a “pointless” MCMC algorithm for this trivial problem:

- Start with an initial value $x_0 \in \{1, 2, 3, 4, 5, 6\}$, e.g. $x_0 = 4$.
- At each iteration t:
  - Roll the die to propose a new value $x' \sim \text{Uniform}\{1, 2, 3, 4, 5, 6\}$.
  - Generate a random number $u \sim \text{Uniform}[0, 1]$.
  - If $u < 0.5$, **accept** x', i.e. set $x_t = x'$.
  - Otherwise, **reject** x' and keep the old value, $x_t = x_{t-1}$.

This produces samples from a Markov chain with transition probabilities:

$$q(x_{t-1} \to x_t) = \frac{1}{2}\mathbf{1}(x_t = x_{t-1}) + \frac{1}{2} \cdot \frac{1}{6} = \begin{cases} \frac{7}{12}, & \text{if } x_t = x_{t-1}, \\ \frac{1}{12}, & \text{if } x_t \neq x_{t-1} \end{cases}$$

Pointless MCMC in Action

Let's simulate a few steps of the "pointless" MCMC algorithm.

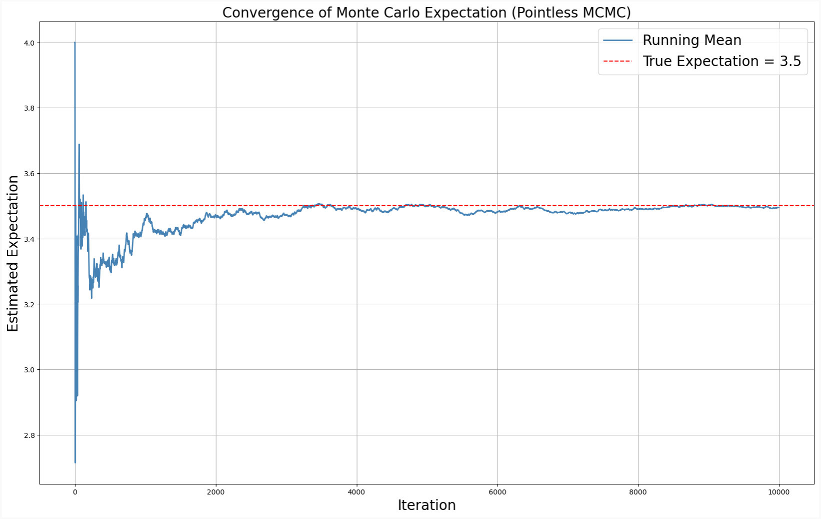
Setup: Start with $x_0 = 4$.

Step	Proposed Roll	u (Uniform(0,1))	Recorded Value (x_t)
1	6	0.234	6 (accepted)
2	3	0.612	6 (rejected)
3	2	0.523	6 (rejected)
4	3	0.125	3 (accepted)
5	2	0.433	2 (accepted)

Resulting samples:

$$x_{0:5} = (4, 6, 6, 6, 3, 2, \ldots)$$

Convergence to the Actual Expectation - Pointless MCMC in Action



Degenerate Example: “Pointless MCMC”

Observation:

- The chain sometimes repeats values due to rejections.
- Samples are **correlated**, even though the target distribution is uniform.

Key insight:

- If you run this chain long enough, you will spend roughly $\frac{1}{6}$ of the time on each outcome.
- The **stationary distribution** is uniform: if we start from a uniform state, either staying there or moving to a uniformly chosen new state keeps the distribution uniform.
- Thus, the stationary distribution of the chain is p (the uniform distribution).
- The property of constructing a chain whose stationary distribution is p is the **key idea behind all MCMC methods**.
- It is “pointless” here because we already know how to generate i.i.d. samples from p. If you can sample directly, you do *not* need MCMC.

Markov Chain Monte Carlo (MCMC)

Goal: Estimate expectations with respect to a distribution $p(x)$ when direct sampling is difficult.

Key idea:

- Construct a **Markov chain** whose **stationary distribution** is $\pi(x) = p(x)$.
  - After sufficient iterations ("burn-in"), samples $x^{(k)}$ approximately follow $p(x)$.
  - Notation: $x^{(1)}$ is the first sampled state, $x^{(2)}$ the second, ..., $x^{(n)}$ the nth.
- Use the dependent Markov chain samples in a Monte Carlo estimator:

$$\mathbb{E}_p[g(X)] \approx \frac{1}{n}\sum_{t=1}^{n} g\left(x^{(t)}\right).$$

- A generalization of the Law of Large Numbers, known as the **Ergodic Theorem**, ensures that as $n \to \infty$:

$$\frac{1}{n}\sum_{t=1}^{n} g\left(x^{(t)}\right) \xrightarrow{\text{a.s.}} \mathbb{E}_p[g(X)].$$

  - Convergence is slower than for i.i.d. samples, since the draws are **correlated**.
  - The variance of the estimator is typically larger than $\mathrm{Var}[g(X)]/n$.
- A widely used method to construct such chains is the Metropolis–Hastings algorithm.

Special Case: Metropolis Algorithm

Metropolis algorithm: Sampling from a continuous target distribution $p(x)$. We assume $p(x)$ can be evaluated up to a normalizing constant:

$$p(x) = \frac{\tilde{p}(x)}{Z}, \quad Z \text{ unknown.}$$

Algorithm:

1. Initialize $x^{(0)}$.
2. Until we get bored:
    - 2.1 Add zero-mean Gaussian noise to generate proposal $\hat{x}^{(t)}$
    $$\hat{x}^{(t)} = x^{(t-1)} + \epsilon, \quad \epsilon \sim N(0, \sigma^2)$$
    - 2.2 Generate $u \sim \text{Uniform}[0, 1]$
    - 2.3 Accept the proposal if
    $$u \le \frac{\tilde{p}(\hat{x}^{(t)})}{\tilde{p}(x^{(t-1)})} \; \frac{\text{probability of proposed}}{\text{probability of current}}$$
    and set $x^{(t)} = \hat{x}^{(t)}$.
    - 2.4 Otherwise, reject the proposal and set $x^{(t)} = x^{(t-1)}$

- Proposals that increase the target density are always accepted.
- Proposals that decrease the target density may be accepted or rejected.
- Under mild conditions (irreducibility, aperiodicity), the chain converges to $p(x)$, but convergence may be slow.
- Works even when the normalizing constant Z is unknown.

Metropolis Algorithm

Algorithm 1 Metropolis Algorithm for Sampling from $p(x)$

```
Require: Initial state $x^{(0)}$, number of iterations $T$, proposal standard deviation $\sigma$
Ensure: Samples $\{x^{(t)}\}_{t=1}^{T}$ approximately distributed according to $p(x)$
 1: Set $x^{(0)}$ as the starting state
 2: for $t = 1$ to $T$ do
 3:     Propose $\hat{x}^{(t)} = x^{(t-1)} + \epsilon$, with $\epsilon \sim N(0, \sigma^2)$
 4:     Generate $u \sim \text{Uniform}(0, 1)$
 5:     if $u \leq \frac{\tilde{p}(\hat{x}^{(t)})}{\tilde{p}(x^{(t-1)})}$ then
 6:         Accept the proposal: $x^{(t)} \leftarrow \hat{x}^{(t)}$
 7:     else
 8:         Reject the proposal: $x^{(t)} \leftarrow x^{(t-1)}$
 9:     end if
10: end for
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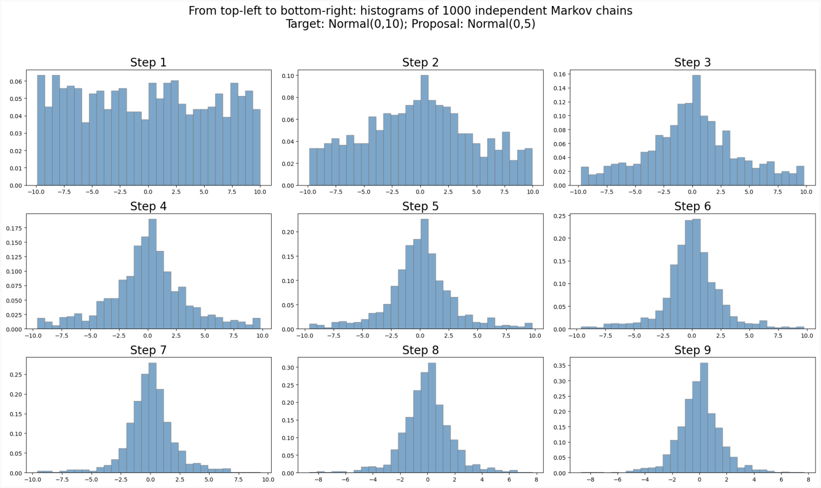
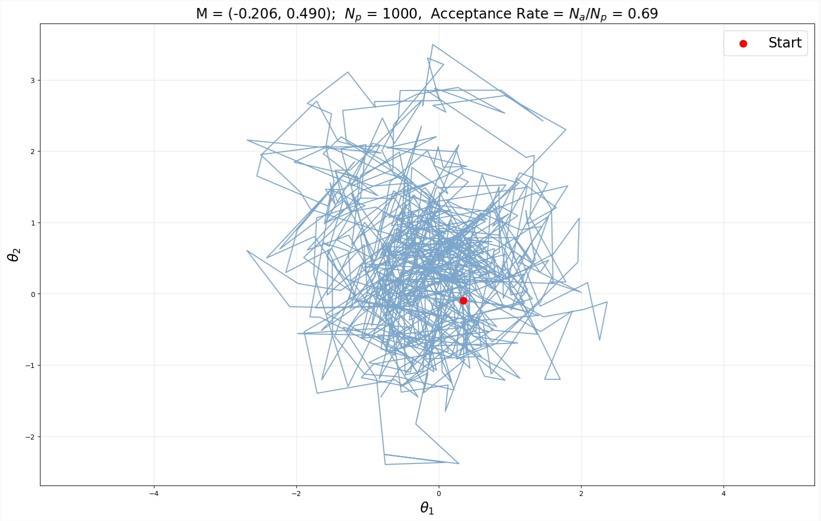
Metropolis Algorithm - Convergence from Uniform to Target Distribution



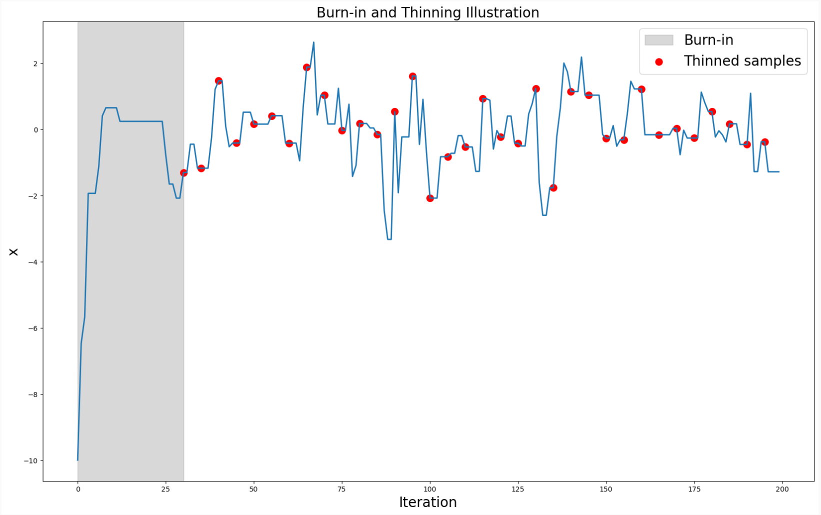
Metropolis Algorithm 2D



MCMC Implementation Issues

- In practice, we often do not *use all* the samples in our Monte Carlo estimates.
- Burn-in: discard the early samples while the chain is far from the stationary distribution.
- Thinning: keep only every k-th sample to reduce autocorrelation between consecutive samples.
- Two common approaches for applying MCMC:
  1. Run a large number of independent chains for a short time and use final states:
     - Highly parallelizable.
     - Effectively an extreme form of thinning: only one sample per chain is used.
     - Must ensure each chain has reached the stationary distribution (burn-in).
  2. Run a single chain for a long time and use states across time:
     - Less concern about burn-in if the chain is sufficiently long.
     - Thinning may be needed to reduce autocorrelation among samples.
- Diagnosing whether the chain has reached the stationary distribution can be difficult in practice.

Visualization of Burn-in and Thinning in MCMC



Homework: Burn-in and Thinning in MCMC

Problem: Consider the Metropolis algorithm for sampling from a target distribution

$$p(x) \propto \exp(-0.05x^2) \quad \text{(Normal(0,10))}.$$

1. Simulate a single Markov chain of length 200, starting from $x_0 = -10$, using a Gaussian random walk proposal with standard deviation 2.
2. Plot the chain over iterations.
3. Highlight the first 30 iterations as burn-in (shaded in gray).
4. Apply thinning by keeping every 5th sample **after burn-in** and mark these samples in red on the plot.
5. In a few sentences, explain why burn-in and thinning are used in MCMC.
6. **Optional / Bonus: Multiple Chains**
   - Run 1000 independent chains, each starting from a random value in [-10,10].
   - Apply burn-in and thinning as before.
   - Combine all thinned samples from all chains and plot a histogram.
   - Comment on how the histogram approximates the target distribution.