

# Markov Chain Monte Carlo

## Theory and Implementation from Scratch

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# Outline

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# What is MCMC?

**Markov Chain Monte Carlo (MCMC)** is a class of algorithms for sampling from probability distributions:

- ▶ **Markov Chain**: A sequence of random samples where each depends only on the previous one
- ▶ **Monte Carlo**: Using random sampling to solve computational problems

MCMC solves a fundamental problem in statistics:

- ▶ How to sample from complex, high-dimensional distributions
- ▶ When direct sampling is impossible or computationally infeasible
- ▶ Essential for Bayesian inference where posterior distributions are often intractable

**Key Insight:** Construct a Markov chain whose stationary distribution is the target distribution we want to sample from.

# Markov Chains

A Markov chain is a sequence of random variables  $X_0, X_1, X_2, \dots$  with the Markov property:

$$P(X_{t+1}|X_t, X_{t-1}, \dots, X_0) = P(X_{t+1}|X_t) \quad (1)$$

## Key Properties for MCMC

- ▶ **Ergodicity:** The chain eventually visits all states with positive probability
- ▶ **Detailed Balance:**  $\pi(x)P(y|x) = \pi(y)P(x|y)$  ensures  $\pi$  is stationary
- ▶ **Convergence:** Under certain conditions, the chain converges to a unique stationary distribution  $\pi$
- ▶ **Irreducibility:** Any state can be reached from any other state

For MCMC, we design the transition kernel  $P(y|x)$  so that  $\pi$  equals our target distribution.

# Metropolis-Hastings Algorithm

## Algorithm Steps:

1. Start with initial value  $x_0$
2. For  $t = 0, 1, 2, \dots$ :
  - ▶ Propose new state  $y \sim q(y|x_t)$  from proposal distribution
  - ▶ Calculate acceptance ratio:

$$\alpha(x_t, y) = \min \left( 1, \frac{\pi(y)q(x_t|y)}{\pi(x_t)q(y|x_t)} \right) \quad (2)$$

- ▶ Accept  $x_{t+1} = y$  with probability  $\alpha$
- ▶ Otherwise, reject and set  $x_{t+1} = x_t$

## Special Cases

- ▶ **Random Walk Metropolis:** Symmetric proposal  $q(y|x) = q(x|y)$
- ▶ **Independence Sampler:** Proposal independent of current state
- ▶ **Gibbs Sampling:** Always accepts (acceptance ratio = 1)

## Gibbs Sampling

Gibbs sampling is a special case of Metropolis-Hastings for multivariate distributions:

For a  $d$ -dimensional distribution  $\pi(x_1, x_2, \dots, x_d)$ :

1. Initialize  $\mathbf{x}^{(0)} = (x_1^{(0)}, x_2^{(0)}, \dots, x_d^{(0)})$
2. For iteration  $t$ :

$$\begin{aligned} x_1^{(t+1)} &\sim \pi(x_1 | x_2^{(t)}, x_3^{(t)}, \dots, x_d^{(t)}) \\ x_2^{(t+1)} &\sim \pi(x_2 | x_1^{(t+1)}, x_3^{(t)}, \dots, x_d^{(t)}) \\ &\vdots \\ x_d^{(t+1)} &\sim \pi(x_d | x_1^{(t+1)}, x_2^{(t+1)}, \dots, x_{d-1}^{(t+1)}) \end{aligned} \tag{3}$$

**Advantages:** No tuning required, always accepts proposals

**Disadvantages:** Requires knowledge of conditional distributions, can be slow for highly correlated variables

# R Implementation - Metropolis-Hastings

```
# Metropolis-Hastings sampler from scratch
metropolis_hastings <- function(target_log_density, initial,
                                 n_samples, proposal_sd = 1) {
  # Initialize storage for samples
  samples <- matrix(0, nrow = n_samples, ncol = length(initial))
  samples[1,] <- initial
  current <- initial
  n_accept <- 0

  # Main MCMC Loop
  for (i in 2:n_samples) {
    # Propose new state (random walk)
    proposal <- current + rnorm(length(current), 0, proposal_sd)

    # Calculate log acceptance ratio
    log_alpha <- target_log_density(proposal) -
      target_log_density(current)

    # Accept or reject
    if (log(runif(1)) < log_alpha) {
      current <- proposal
      n_accept <- n_accept + 1
    }
    samples[i,] <- current
  }

  list(samples = samples, accept_rate = n_accept / n_samples)
}
```

# R Implementation - Gibbs Sampling

```
# Gibbs sampler for bivariate normal distribution
gibbs_sampler <- function(n_samples, mu1 = 0, mu2 = 0,
                           sigma1 = 1, sigma2 = 1, rho = 0.8) {
  # Initialize storage
  samples <- matrix(0, nrow = n_samples, ncol = 2)
  samples[1,] <- c(0, 0) # Initial values

  # Conditional distribution parameters
  for (i in 2:n_samples) {
    # Sample x1 / x2
    mu_cond1 <- mu1 + rho * sigma1/sigma2 * (samples[i-1, 2] - mu2)
    sigma_cond1 <- sqrt((1 - rho^2) * sigma1^2)
    samples[i, 1] <- rnorm(1, mu_cond1, sigma_cond1)

    # Sample x2 / x1
    mu_cond2 <- mu2 + rho * sigma2/sigma1 * (samples[i, 1] - mu1)
    sigma_cond2 <- sqrt((1 - rho^2) * sigma2^2)
    samples[i, 2] <- rnorm(1, mu_cond2, sigma_cond2)
  }

  return(samples)
}
```

# R Implementation - Example Application

```
# Example: Sampling from a mixture of Gaussians
mixture_log_density <- function(x) {
  # Log density of 0.3*N(-2,1) + 0.7*N(3,1.5)
  comp1 <- 0.3 * dnorm(x, -2, 1)
  comp2 <- 0.7 * dnorm(x, 3, 1.5)
  return(log(comp1 + comp2))
}

# Run MCMC
set.seed(123)
result <- metropolis_hastings(mixture_log_density,
                               initial = 0,
                               n_samples = 10000,
                               proposal_sd = 2)

# Print diagnostics
cat("Acceptance rate:", round(result$accept_rate, 3), "\n")
```

Acceptance rate: 0.671

```
cat("Sample mean:", round(mean(result$samples[5001:10000]), 3), "\n")
```

Sample mean: 1.279

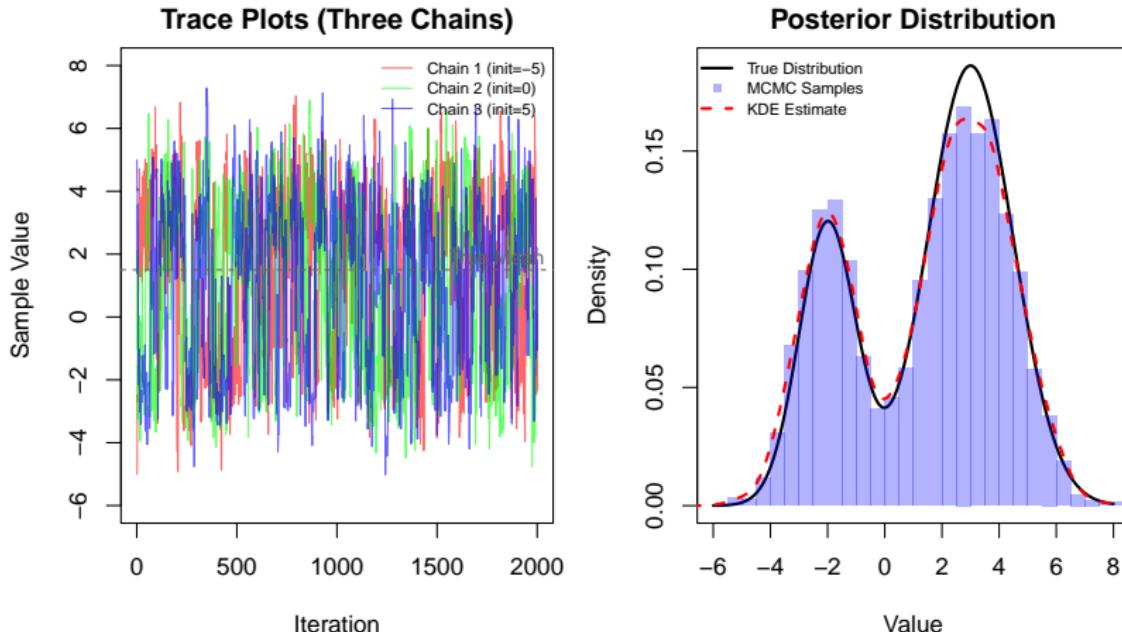
```
cat("Sample std dev:", round(sd(result$samples[5001:10000]), 3), "\n")
```

Sample std dev: 2.791

```
# True theoretical values
true_mean <- 0.3*(-2) + 0.7*3  # 1.5
true_var <- 0.3*(1 + 4) + 0.7*(1.5^2 + 9) - 1.5^2  # 8.475
cat("True mean:", true_mean, "\n")
```

True mean: 1.5

# Visualization of MCMC Convergence



- ▶ Left: Three chains with different initial values converge to the same distribution
- ▶ Right: MCMC samples accurately approximate the true mixture distribution
- ▶ Burn-in period ( 1000 iterations) allows chains to reach stationarity

# Applications and Takeaways

## Key Applications

- ▶ **Bayesian Inference:** Sampling from posterior distributions
- ▶ **Financial Modeling:** Option pricing, risk assessment, portfolio optimization
- ▶ **Machine Learning:** Bayesian neural networks, latent variable models
- ▶ **Physics:** Statistical mechanics, quantum field theory simulations
- ▶ **Genetics:** Phylogenetic tree reconstruction, population genetics

## Takeaways

- ▶ MCMC enables sampling from complex distributions where direct methods fail
- ▶ Metropolis-Hastings provides a general framework: accept/reject based on  $\alpha = \min\left(1, \frac{\pi(y)q(x|y)}{\pi(x)q(y|x)}\right)$
- ▶ Convergence diagnostics are crucial: check trace plots, autocorrelation, and  $\hat{R}$
- ▶ Trade-off between exploration (large steps) and acceptance rate
- ▶ Modern variants (HMC, NUTS) improve efficiency for high-dimensional problems