Lecture 3: Markov Chain Monte Carlo

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Outline

1. Introduction of MCMC
2. Metropolis–Hastings Algorithm
3. Gibbs Sampler
4. Hamiltonian Monte Carlo Method
5. References

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Markov Chain Monte Carlo (MCMC)

- Revolutionized statistics and scientific computation
- Expanding the range of possible distributions that we can simulate from, including joint distributions in high dimensions
- Basic idea: build your own Markov chain $(X_0, X_1, \ldots)$ so that the desired distribution π is the stationary distribution of the chain.
- Sampling from distribution π (running the chain for a long time and then sampling)
- Further do sample mean & sample variance & other sample functions
- Connections to optimization

Sampling $\longleftrightarrow$ optimization

MCMC Method

- Forward engineering(Analysis): given the transition matrix P, find the stationary distribution of Markov chain.
- Reverse engineering(Design): given a distribution π that we want to simulate, we will engineer a Markov chain whose stationary distribution is π. Then run this engineered Markov chain for a long time, the distribution of the chain will approach π.

MCMC Method

- Markov Chain Monte Carlo (MCMC) is a remarkable methodology, which utilizes Markov sequences to effectively simulate from what would otherwise be intractable distributions.
- All MCMC algorithms construct reversible (time-reversible) Markov chain: detailed balance equations help us.
- Two most widely used algorithms: Metropolis-Hastings & Gibbs Sampling

Theory Justification: Strong Law of Large Numbers for Markov Chains

Theorem

Assume that $X_0, X_1, \cdots$ is an ergodic Markov chain with stationary distribution π. Let r be a bounded, real-valued function. Let X be a random variable with distribution π. Then, with probability 1,

$$\lim_{n\to\infty} \frac{r(X_1) + \cdots + r(X_n)}{n} = E(r(X)).$$

where $E(r(X)) = \sum_j r(j)\pi_j$.

Example: Bob's Lunch

$\pi P = \pi$

Stationary π: distribution

$\pi_1 = \pi_2 = \frac{1}{5}$;
$\pi_3 = \frac{3}{20}$;
$\pi_4 = \frac{9}{20}$;

Bob's daily lunch choices at the cafeteria are described by a Markov chain with transition matrix

$$P = \begin{array}{c} \\ \text{Yogurt} \\ \text{Salad} \\ \text{Hamburger} \\ \text{Pizza} \end{array} \begin{array}{c} \begin{array}{cccc} \text{Yogurt} & \text{Salad} & \text{Hamburger} & \text{Pizza} \end{array} \\ \begin{pmatrix} 0 & 0 & 1/2 & 1/2 \\ 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 0 & 1/2 \\ 1/4 & 1/4 & 0 & 1/2 \end{pmatrix} \end{array}$$

1 2 3 4

Yogurt costs \$3.00, hamburgers cost \$7.00, and salad and pizza cost \$4.00 each. Over the long term, how much, on average, does Bob spend for lunch?

Solution

1°. X = state of m.c.; $X \in$ {"Yogurt", "Salad", "Hamburger", "pizza"}

$r(X)$: food rice

$$r(X) = \begin{cases} 3 & \text{if } X = \text{"Yogurt"} \\ 4 & \text{if } X = \text{"Salad" or "pizza"} \\ 7 & \text{if } X = \text{"Hamburger"} \end{cases}$$

2°. n : days for lunch of m.c. $\{X_t\}$. ergodic (irreducible; aperiodic; finite state;)

$$\lim_{n\to\infty} \frac{1}{n}[r(X_1) + r(X_2) + \cdots + r(X_n)] \overset{SLLN}{=} E[r(X)] = \sum_x r(x)\pi(x)$$

3°. Stationary distribution of m.c. $\pi P = \pi$; $\pi = (\frac{1}{5}, \frac{1}{5}, \frac{3}{20}, \frac{9}{20})$

(Y, S, H, P)

4°. $\sum_x r(x)\pi(x) = 3 \cdot \frac{1}{5} + 4 \cdot \frac{1}{5} + 7 \cdot \frac{3}{20} + 4 \cdot \frac{9}{20}$

$= 4.25$ \$ per day

Example: Binary Sequences with No Adjacent 1s

$m=2$; there are $2^m = 2^2 = 4$ binary sequences.

$\frac{1}{3}$ 00 ✓
$\frac{1}{3}$ 01 ✓
$\frac{1}{3}$ 10 ✓
11 ✗

good sequences.

$\frac{1}{3}\cdot 0 + \frac{1}{3}\cdot 1 + \frac{1}{3}\cdot 1 = \frac{2}{3}$

$m=100$; $2^{100} \approx 10^{30}$ binary sequences; $\approx 10^{21}$ good sequences.

Consider sequences of length m consisting of 0s and 1s. Call a sequence good if it has no adjacent 1s. What is the expected number of 1s in a good sequence if all good sequences are equal likely?

1°. Construct an ergodic M.C. { state : good sequence. state space : good sequences.

desired stationary distribution π : uniform distribution. [# of good sequences $= C$] $[\frac{1}{C}, \frac{1}{C}, \frac{1}{C}, \dots \frac{1}{C}]$

2°: X : state (good sequences). $X \sim \pi$

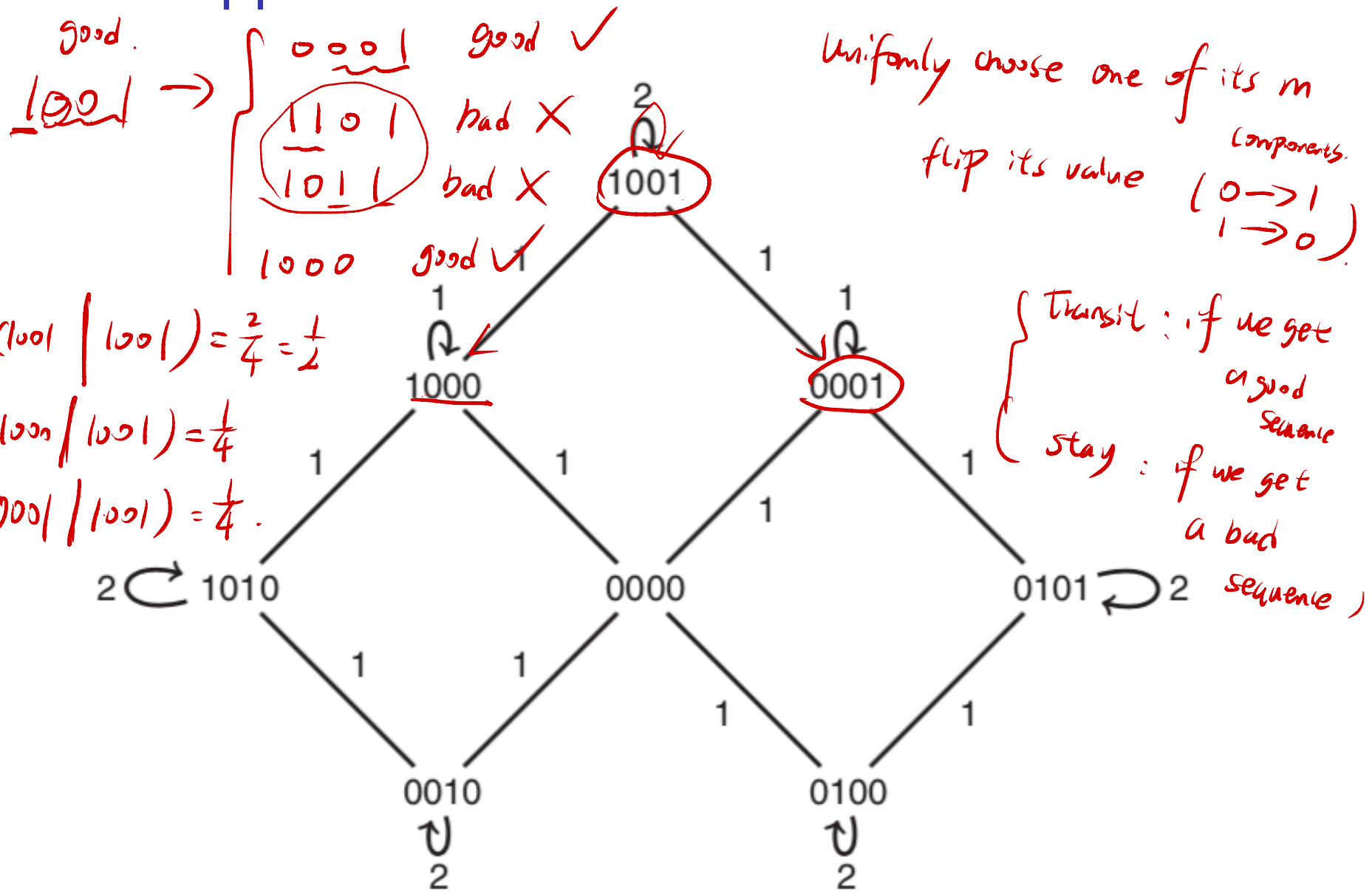
$r(X)$: # of "1" in state X.

$E[r(X)] \approx \frac{1}{n}[r(X_1) + r(X_2) + \cdots + r(X_n)]$ finite n

MCMC Approach

$n = 4$

Design P (transition matrix) Prob.



MCMC Approach

1°. DTMC
finite state $< 2^m$.
ergodic { irreducible, aperiodic.
a

length-m
a → 0000 → b
at most m-1 flip
at most m-1 flip
$a \rightleftarrows b$ $\leq 2(m-1)$ steps

2°. a → b. iff $dist^H(a,b) = 1$
Hamming distance.
$P_{a,b} = \frac{1}{m}$ $a \neq b$.

0000 / 1000 $dist^H(\cdot) = 1$
0001 / 1000 $dist^H(\cdot) = 2$

Solve detailed balance equation DBE.

$\pi_i P_{i,j} = \pi_j \cdot P_{j,i}$, $i \neq j$, $dist^H(i,j) = 1$ | C = # of good states.

$P_{i,j} = P_{j,i} = \frac{1}{m} \Rightarrow \pi_i = \pi_j \ \forall i \neq j \Rightarrow \pi_i = \frac{1}{C}$

Solution of DBE: uniform distribution (π) $\Rightarrow$ Stationary distribution of M.C.

3°. $m = 100$; theory $\mu = 27.7921$.
Sample $n = 100000$; MCMC $\hat{\mu} = 27.833$.

HW: CTMC?

MCMC Approach

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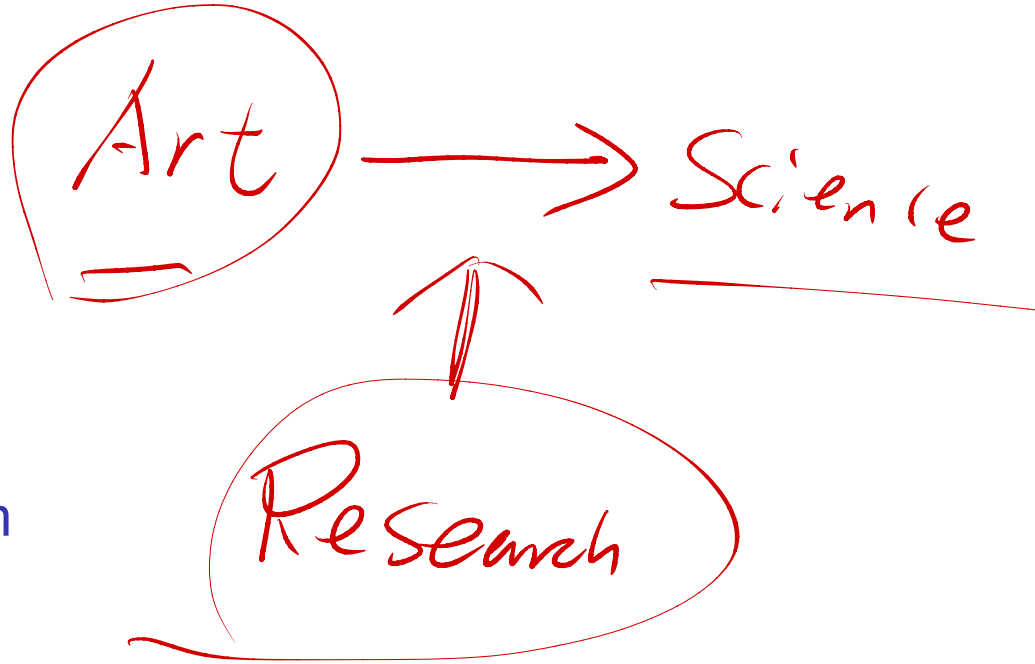


Basic Idea

- Proposed by Nicholas Metropolis in 1953 & further developed by Wilfred Keith Hastings in 1970.
- Start with any irreducible Markov chain on the state space of interest
- Then modify it into a new Markov chain with desired stationary distribution
- Modification: moves are proposed according to the original chain, but the proposal may or may not be accepted.
- Art: choice of the probability of accepting the proposal

Algorithm for DTMC

Let $\pi = (\pi_1, ..., \pi_M)$ be a desired stationary distribution on state space $\{1, ..., M\}$. Assume that $\pi_i > 0$ for all i (if not, just delete any states i with $s_i = 0$ from the state space). Suppose that $P = (p_{ij})$ is the transition matrix for a Markov chain on state space $\{1, ..., M\}$. Intuitively, P is a Markov chain that we know how to run but that doesn't have the desired stationary distribution. Now we will modify P to construct a Markov chain.

- Use the original transition probabilities p_{ij} to propose where to go next
- Then accept the proposal with probability a_{ij}
- Staying in the current state in the event of a rejection.
- Normalization of π does not need to be known.

Algorithm Metropolis-Hastings

Require:

Stationary distribution $\pi = (\pi_1, ..., \pi_M)$;

Original transition matrix $P = (p_{ij})$;

State X_0 (chosen randomly or deterministically);

Ensure:

Modified transition matrix $P' = (p'_{ij})$;

1: **repeat**

2: If $X_n = i$, propose a new state j using the transition probabilities in the ith row of the original transition matrix P;

3: Compute the acceptance probability $a_{ij} = \min\left(\frac{\pi_j p_{ji}}{\pi_i p_{ij}}, 1\right)$;

4: Flip a coin that lands Heads with probability a_{ij};

5: If the coin lands Heads, accept the proposal (i.e., go to j), setting $X_{n+1} = j$. Otherwise, reject the proposal (i.e., stay at i), setting $X_{n+1} = i$;

6: **until** Convergence;

7: **return** P';

Metropolis–Hastings Algorithm

1^0. irreducible ✓ (from irreducible proposal M.C.)

aperiodic ✓

2^0. detailed balance equation

$\pi_i P_{i,j}' \overset{\checkmark}{=} \pi_j P_{j,i}'$ | $P_{i,j}' = P_{i,j} \cdot a_{i,j}$

Theorem

The sequence $X_0, X_1, \cdots$ constructed by the Metropolis–Hastings algorithm is a reversible Markov chain with stationary distribution π.

LHS: $\pi_i P_{i,j}' = \pi_i \cdot P_{i,j} a_{i,j} = \pi_i P_{i,j} \cdot \min\left(\frac{\pi_j P_{j,i}}{\pi_i P_{i,j}}, 1\right)$

$= \min(\pi_j P_{j,i}, \pi_i P_{i,j})$ $\quad \min(A,B)$

RHS: $\pi_j P_{j,i}' = \pi_j P_{j,i} \cdot a_{j,i} = \pi_j P_{j,i} \cdot \min\left(\frac{\pi_i P_{i,j}}{\pi_j P_{j,i}}, 1\right)$

$= \min(\pi_i P_{i,j}, \pi_j P_{j,i})$ $\quad \min(B,A)$

Remarks

- The exact form of π is not necessary to implement Metropolis–Hastings. The algorithm only uses ratios of the form $\frac{\pi_j}{\pi_i}$. Thus, π needs only to be specified up to proportionality.
- If the proposal transition matrix P is symmetric, $a_{ij} = \min\left(\frac{\pi_j}{\pi_i}, 1\right)$.
- The algorithm works for any irreducible proposal chain. Thus, the user has wide latitude to find a proposal chain that is efficient in the context of their problem.
- Under some conditions (e.g. finite state), the resulting Metropolis–Hastings chain is also ergodic with limiting(stationary) distribution π.

Remarks

- The generated sequence $X_0, X_1, \ldots, X_n$ gives an approximate sample from π.
- If the chain requires many steps to get close to stationarity, there may be initial bias.
- Burn-in: the practice of discarding the initial iterations and retaining $X_m, X_{m+1}, \ldots, X_n$, for some m.
- The strong laws of large numbers for Markov chains:

$$\lim_{n\to\infty} \frac{r(X_m) + \cdots + r(X_n)}{n - m + 1} = E(r(X)) = \sum_x r(x)\pi_x.$$

Example: Power-law Distribution

Power-law distributions are positive probability distributions of the form $\pi_i \propto i^S$, for some constant S. Unlike distributions with exponentially decaying tails (e.g., Poisson, geometric, exponential, normal), power-law distributions have *fat tails*, and thus are often used to model skewed data. Let

$$\pi_i = \frac{i^{-3/2}}{\sum_{k=1}^{\infty} k^{-3/2}}, \text{ for } i = 1, 2, \cdots$$

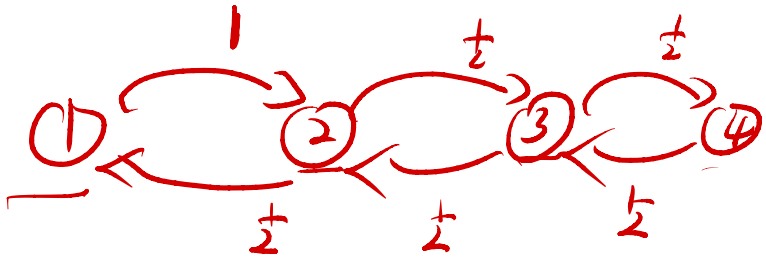
Implement a Metropolis–Hastings algorithm to simulate from $\boldsymbol{\pi}$.

Solution

1°. State space : $\{1, 2, \dots \infty\}$

State = positive integer.

Proposal Markov chain: Simple symmetric random walk on the positive integer with one reflecting bound.



irreducible M.C.

$$P_{i,j} = \begin{cases} \frac{1}{2} & \text{if } j = i \pm 1, i \geq 2 \\ 1 & \text{if } i = 1, j = 2 \\ 0 & \text{otherwise.} \end{cases}$$

2°. $\pi_i \propto i^{-\frac{3}{2}}$

the acceptance prob.

$$a_{i,j} = \min\left(\frac{\pi_j P_{j,i}}{\pi_i P_{i,j}}, 1\right)$$

$$= \min\left(\frac{j^{-\frac{3}{2}} \cdot P_{j,i}}{i^{-\frac{3}{2}} \cdot P_{i,j}}, 1\right)$$

Solution

$$a_{1,2} = \min\left(\frac{\pi_2 P_{2,1}}{\pi_1 P_{1,2}}, 1\right) = \min\left(\frac{2^{-\frac{3}{2}} \cdot 2 \cdot 1}{1^{-\frac{3}{2}} \cdot 1}, 1\right)$$

$$= 2^{-\frac{5}{2}}$$

$$a_{2,1} = \min\left(2^{\frac{5}{2}}, 1\right) = 1$$

3°. $i, j \geq 2$ $\Rightarrow$ $a_{i,i+1} = \min\left(\frac{(i+1)^{-\frac{3}{2}} \cdot}{i^{-\frac{3}{2}} \cdot}, 1\right)$

$P_{i,j} = P_{j,i} = \frac{1}{2}$

$$= \left(\frac{i}{i+1}\right)^{\frac{3}{2}}$$

$$a_{i+1,i} = \min\left(\frac{i^{-\frac{3}{2}}}{(i+1)^{-\frac{3}{2}}}, 1\right)$$

$$= \min\left(\left(\frac{i+1}{i}\right)^{\frac{3}{2}}, 1\right) = 1$$

Solution

TABLE 5.1 Comparison of Markov chain Monte Carlo Estimates with Exact Probabilities for Power-Law Distribution

i	1	2	3	4	5	6	7	8	≥ 9
Simulation	0.389	0.137	0.075	0.048	0.034	0.026	0.021	0.017	0.252
Exact	0.383	0.135	0.074	0.048	0.034	0.026	0.021	0.017	0.262

Example: Zipf Distribution Simulation

Let $M \geq 2$ be an integer. An r.v. X has the *Zipf distribution* with parameter $a > 0$ if its PMF is

$$P(X = k) = \frac{1/k^a}{\sum_{i=1}^{M} (1/j^a)},$$

for $k = 1, 2, ..., M$ (and 0 otherwise). This distribution is widely used in linguistics for studying frequencies of words.

Create a Markov chain $X_0, X_1, ...$ whose stationary distribution is the Zipf distribution, and such that $|X_{n+1} - X_n| \leq 1$ for all n. Your answer should provide a simple, precise description of how each move of the chain is obtained, i.e., how to transition from X_n to X_{n+1} for each n.

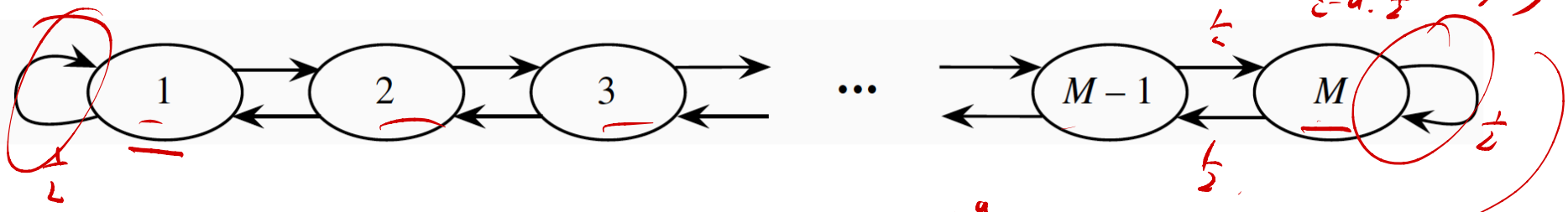
Solution

1°. Proposal Markov chain: State: $1, 2, \dots, M$

State space: $\{1, 2, \dots, M\}$.

simple random walk: $P_{i,j} = \begin{cases} \frac{1}{2} & \text{iff } |i-j| \le 1 \\ 0 & \text{otherwise.} \end{cases}$

2°. $|i-j| \le 1$, $a_{i,j} = \min\left(\frac{\pi_j P_{j,i}}{\pi_i P_{i,j}}, 1\right) = \min\left(\frac{j^{-a} \cdot \frac{1}{2}}{i^{-a} \cdot \frac{1}{2}}, 1\right)$



$= \min\left(\frac{i^a}{j^a}, 1\right)$

$a_{1,1} = a_{M,M} = 1$

$a_{i,i+1} = \min\left(\frac{i^a}{(i+1)^a}, 1\right) = \left(\frac{i}{i+1}\right)^a$, $1 \le i \le M-1$

$a_{i,i-1} = \min\left(\left(\frac{i}{i-1}\right)^a, 1\right) = 1$, $2 \le i \le M$

Solution

Example: Knapsack Problem

- m treasures with labels from 1 to m, where the jth treasure is worth g_j gold pieces and weighs w_j pounds.
- The maximum weight we can carry is w pounds.
- We must choose a vector $x = (x_1, \ldots, x_m)$, where x_j is 1 if we choose the jth treasure and 0 otherwise, such that the total weight of the treasures j with $x_j = 1$ is at most w.
- Let C be the space of all such vectors, so C consists of all binary vectors $(x_1, \ldots, x_m)$ with $\sum_{j=1}^{m} x_j w_j \leq w$.
- We wishes to maximize the total worth of the treasure we takes.
- Finding an optimal solution is an extremely difficult problem, known as the knapsack problem, which has a long history in computer science.
- A brute force solution would be completely infeasible in general. How about MCMC?

Example: Knapsack Problem

(a) State $x = (x_1, \ldots, x_m)$; State space $C = \{x : \sum_{j=1}^{m} x_j w_j \le w\}$

if $x \to y$; $P_{x,y} = \frac{1}{m}$;

$y \to x$; $P_{y,x} = \frac{1}{m}$;

$\pi P = \pi$ ✓ (π uniform distribution)

(a) Consider the following Markov chain. Start at $(0, 0, \ldots, 0)$. One move of the chain is as follows. Suppose the current state is $x = (x_1, \ldots, x_m)$. Choose a uniformly random J in $\{1, 2, \ldots, m\}$, and obtain y from x by replacing x_J with $1 - x_J$ (i.e., toggle whether that treasure will be taken). If y is not in C, stay at x; if y is in C, move to y. Show that the uniform distribution over C is stationary for this chain.

(b) Show that the chain from (a) is irreducible, and that it may or may not be aperiodic (depending on $w, w_1, \ldots, w_m$).

(b) $\forall$ states x, y.

$x \longleftrightarrow \{0, 0, \ldots, 0\} \longrightarrow y$

at most m steps. at most m steps.

$x \rightleftarrows y$ at most $2m$ steps.

Solution

Periodicity : $w, w_1, \dots w_n$

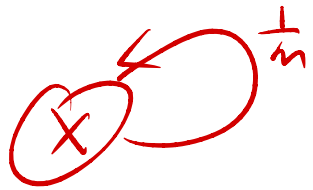
1^0. $w_1 + w_2 + \cdots + w_n < W$

All binary vectors of length-n are allowed.

$(0, 0, \dots, 0)$ period of 2 (pick up + drop)

2^0. $w_1 > W$.

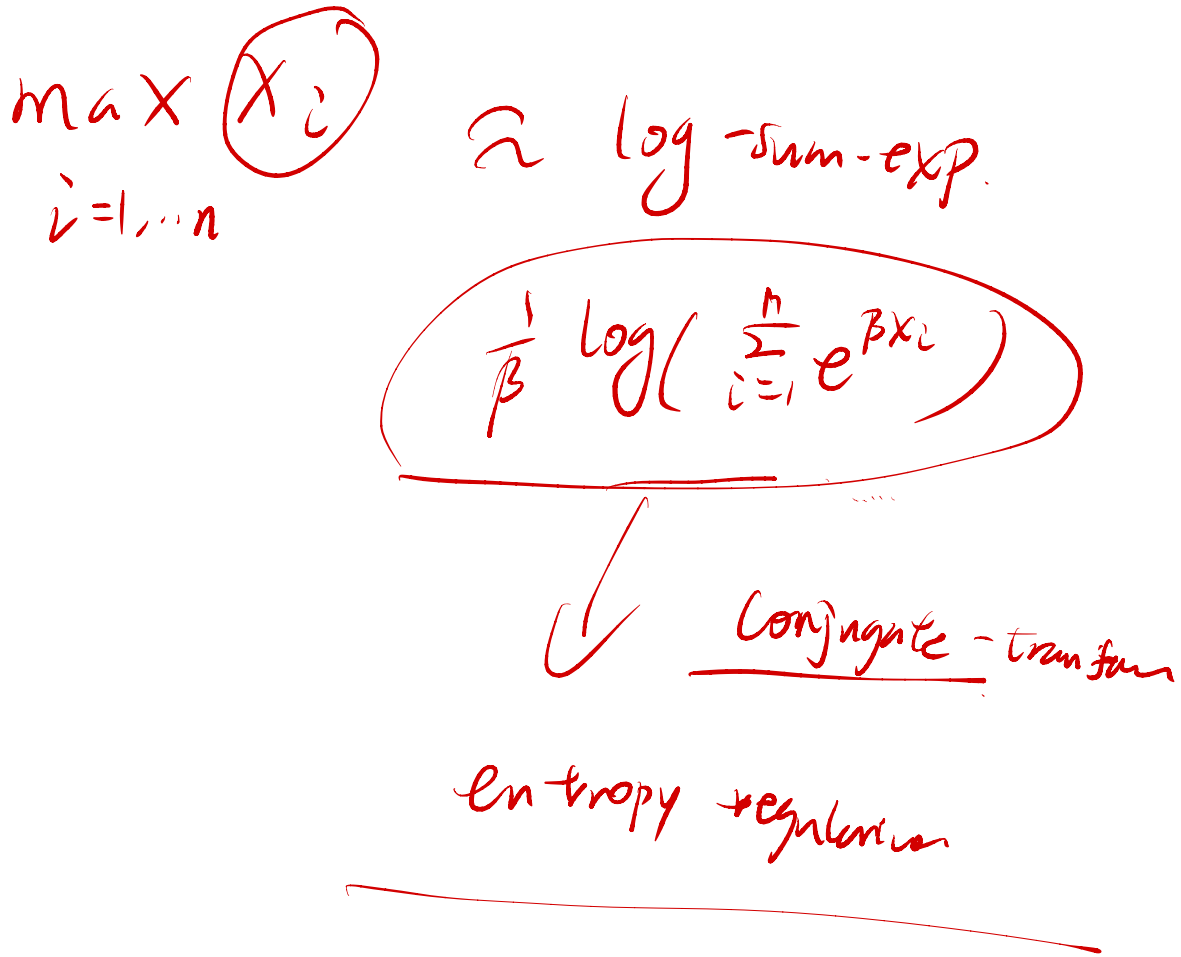
$(0, x_2, \dots x_n)$ (x)



$\frac{1}{n} \rightarrow (1, x_2, \dots x_n)$ (y) $\notin C$.

aperiodic

Solution


max x_i
$i = 1, \dots n$
$\approx$ log-sum-exp
$\frac{1}{\beta} \log\left(\sum_{i=1}^{n} e^{\beta x_i}\right)$
Conjugate - transform
entropy regularization

Example: Knapsack Problem

(c) The chain from (a) is a useful way to get approximately *uniform* solutions, but Bilbo is more interested in finding solutions where the value (in gold pieces) is high. In this part, the goal is to construct a Markov chain with a stationary distribution that puts much higher probability on any particular high-value solution than on any particular low-value solution. Specifically, suppose that we want to simulate from the distribution

$$s(x) \propto e^{\beta V(x)},$$

where $V(x) = \sum_{j=1}^{m} x_j g_j$ is the value of x in gold pieces and β is a positive constant. The idea behind this distribution is to give exponentially more probability to each high-value solution than to each low-value solution. Create a Markov chain whose stationary distribution is as desired.

Solution

$\beta > 0$

1°. desired distribution $\pi(x) \propto e^{\beta V(x)}$, $V(x) = \sum_{j=1}^{m} x_j \cdot g_j$

2°. Proposal Markov chain in Part (a)

acceptance prob.

$$a_{x,y} = \min\left(\frac{\pi_y P_{y,x}}{\pi_x P_{x,y}}, 1\right)$$

$$= \min\left(\frac{\pi_y}{\pi_x}, 1\right) = \min\left[e^{\beta[U(y)-U(x)]}, 1\right]$$

$\pi(x) \propto e^{\beta V(x)}$ $\quad e^{(\cdot)}$

$\pi(x) \propto F[U(x)]$

Solution

$\pi(x) \propto e^{\beta V(x)} \Rightarrow \pi(x) = \frac{e^{\beta V(x)}}{\sum_{y \in C} e^{\beta V(y)}}, \forall x \in C.$

1°. $\beta \to 0$; $\pi(x) \to \frac{1}{|C|}$, $|C|$: size of C.

Uniform distribution.

(c) We can apply Metropolis-Hastings using the chain from (a) to make proposals. Start at $(0, 0, \ldots, 0)$. Suppose the current state is $x = (x_1, \ldots, x_m)$. Then:

1. Choose a uniformly random J in $\{1, 2, \ldots, m\}$, and obtain y from x by replacing x_J with $1 - x_J$.

2. If y is not in C, stay at x. If y is in C, flip a coin that lands Heads with probability $\min\left(1, e^{\beta(V(y)-V(x))}\right)$. If the coin lands Heads, go to y; otherwise, stay at x.

2°. $\beta \to \infty$; $V(x^*) > V(x)$, $\forall x \neq x^*$, $x^* \in C$ $\quad \pi(x) \to \begin{cases} 1 & \text{if } x = x^* \\ 0 & \text{otherwise.} \end{cases}$

$\pi(x^*) = \frac{e^{\beta V(x^*)}}{\sum_{y \neq x^*} e^{\beta V(y)} + e^{\beta V(x^*)}} = \frac{1}{\sum_{y \neq x^*} e^{\beta [V(y) - V(x^*)]} + 1} \to \frac{1}{0+1} = 1$

$\pi(x) \to 0$, $x \neq x^*$;

Solution

$a_{x,y} = \min(1, e^{\beta[U(y)-U(x)]})$.

1°. $\beta \gg 1$. if x is local optimal, y: neighbor states of x, $U(y) < U(x)$

$\beta \to \infty$ $a_{x,y} = 0$;

Bruce Hajek 1988.

$T_t = \frac{c}{\log(t+1)}$;

$\beta_t = \log(t+1)$;

stuck in local optimal.

slow convergence

} exploitation

2°. $\beta \ll 1$. $\beta \to 0$, $a_{x,y} = 1$

far from optimal.

Fast convergence

} exploration

β : Small → Large exploitation

explore state space

$\beta = \frac{1}{\text{Temperature}}$.

T:

Annealing

Simulated

Discrete Time, Continuous State Space

- MH algorithm can also be used in the discrete time, continuous state case (Discrete Markov Process), when π is a probability density function.
- For a continuous state space $\mathcal{S}$, a transition *function* replaces the transition matrix.
- $f_{x,y} = f_{X_{n+1}|X_n}(y|x)$ is the one-step transition probability density from state x to state y.
- Irreducible condition: $f_{x,y} > 0, \forall x, y \in \mathcal{S}$
- Compute the acceptance probability:

$$a_{i,j} = \min\left(\frac{\pi_j f_{j,i}}{\pi_i f_{i,j}}, 1\right).$$

- π_i: pdf in state i
- $f_{i,j}$: one-step transition probability density from state i to state j

Example: Beta Simulation

1°. PDF $f(x) = \frac{1}{B(a,b)} x^{a-1}(1-x)^{b-1}$, $0<x<1$, $a>0$, $b>0$

Suppose that we want to generate $W \sim \mathrm{Beta}(a, b)$. What we have available are i.i.d. $\mathrm{Unif}(0, 1)$ r.v.s. How can we generate W which is *approximately* $\mathrm{Beta}(a, b)$ if a and b are any positive real numbers, with the help of a Markov chain on the continuous state space $(0, 1)$?

HW: Acceptance-Rejection Method vs. MCMC(MH)

2°.

Solution

Solution

1°. Proposal M.P.: independent sampler. (degeneration of M.P.)

Unif(0,1) r.v.

2°. Acceptance prob. $\min\left(\frac{z_u \cdot f_w}{z_w \cdot f_u}, 1\right)$

$w \to u$

Let W_0 be any starting state, and generate a chain $W_0, W_1, \ldots$ as follows. If the chain is currently at state w (a real number in $(0,1)$), then:

1. Generate a proposal u by drawing a Unif$(0,1)$ r.v.
2. Accept the proposal with probability $\min\left(\frac{u^{a-1}(1-u)^{b-1}}{w^{a-1}(1-w)^{b-1}}, 1\right)$. If the proposal is accepted, go to u; otherwise, stay at w.

$= \min\left(\frac{z_u}{z_w}, 1\right)$

$= \min\left(\frac{u^{a-1}(1-u)^{b-1}}{w^{a-1}(1-w)^{b-1}}, 1\right)$

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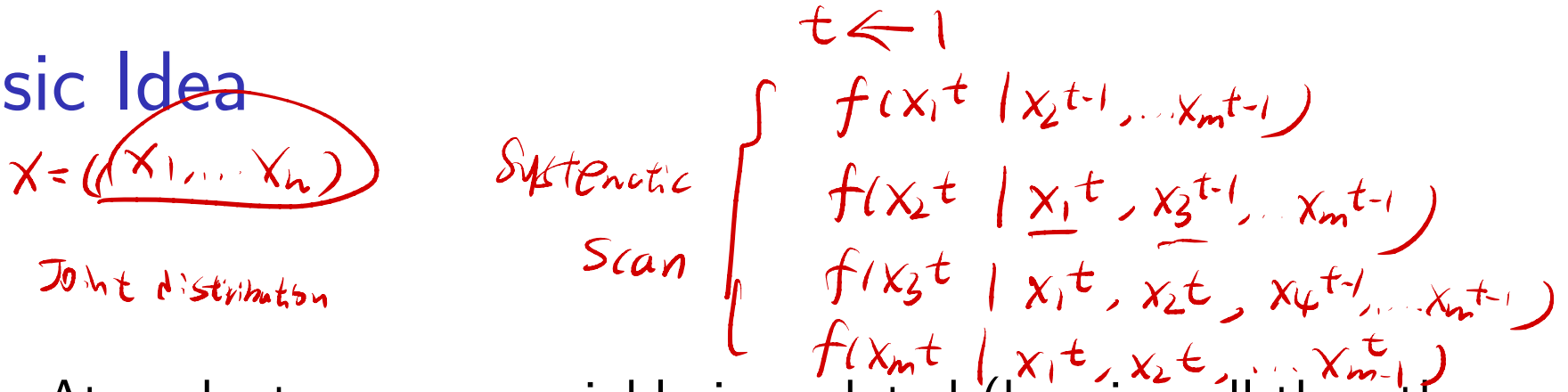
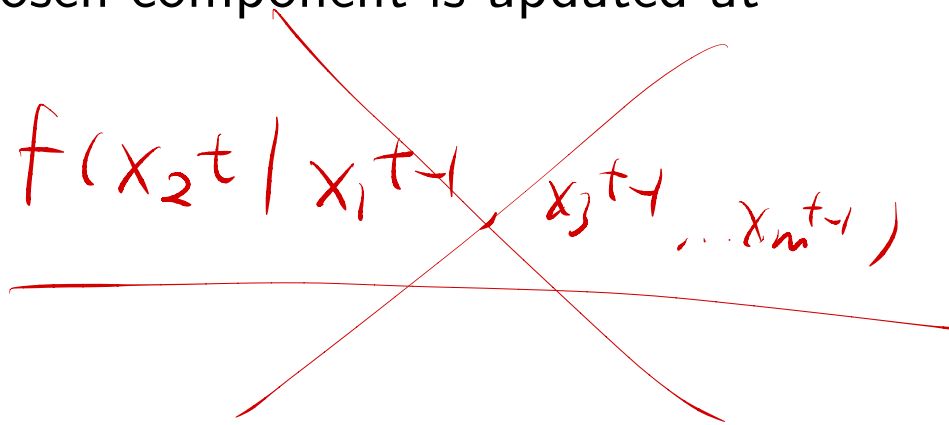
Basic Idea

- Proposed by brothers Stuart and Donald Geman in 1984.
- Named after the physicist Josiah Willard Gibbs, in reference to an analogy between the sampling algorithm and statistical physics.
- Obtaining approximate draws from a joint distribution, based on sampling from conditional distributions one at a time
- Especially useful in problems where these conditional distributions are pleasant to work with.

Basic Idea



- At each stage, one variable is updated (keeping all the other variables fixed) by drawing from the conditional distribution of that variable given all the other variables.
- Two major kinds of Gibbs sampler:
  - systematic scan: the updates sweep through the components in a deterministic order.
  - random scan: a randomly chosen component is updated at each stage.



Algorithm: Systematic Scan Gibbs Sampler

Let X and Y be discrete r.v.s with joint PMF $p_{X,Y}(x, y) = P(X = x, Y = y)$. We wish to construct a two-dimensional Markov chain (X_n, Y_n) whose stationary distribution is $p_{X,Y}$. The systematic scan Gibbs sampler proceeds by updating the X-component and the Y-component in alternation. If the current state is $(X_n, Y_n) = (x_n, y_n)$, then we update the X-component while holding the Y-component fixed, and then update the Y-component while holding the X-component fixed.

Algorithm Systematic Scan Gibbs Sampler

Require:

Joint PMF $p_{X,Y}$;

Initial state (X_0, Y_0);

Ensure:

Two-dimensional Markov chain (X_n, Y_n);

1: **repeat**

2: Draw a value x_{n+1} from the conditional distribution of X given $Y = y_n$, and set $X_{n+1} = x_{n+1}$;

3: Draw a value y_{n+1} from the conditional distribution of Y given $X = x_{n+1}$, and set $Y_{n+1} = y_{n+1}$;

4: **return** (X_{n+1}, Y_{n+1});

5: **until** $n \geq N$;

Algorithm: Random Scan Gibbs Sampler

As above, let X and Y be discrete r.v.s with joint PMF $p_{X,Y}(x, y)$. We wish to construct a two-dimensional Markov chain (X_n, Y_n) whose stationary distribution is $p_{X,Y}$. Each move of the random scan Gibbs sampler picks a uniformly random component and updates it, according to the conditional distribution given the other component.

Algorithm Random scan Gibbs sampler

Require:

Joint PMF $p_{X,Y}$;

Initial state (X_0, Y_0);

Ensure:

Two-dimensional Markov chain (X_n, Y_n);

1: **repeat**

2: Choose which component to update, with equal probabilities;

3: If the X-component was chosen, draw a value x_{n+1} from the conditional distribution of X given $Y = y_n$, and set $X_{n+1} = x_{n+1}, Y_{n+1} = y_n$. Similarly, if the Y-component was chosen, draw a value y_{n+1} from the conditional distribution of Y given $X = x_n$, and set $X_{n+1} = x_n$, $Y_{n+1} = y_{n+1}$;

4: **return** (X_{n+1}, Y_{n+1});

5: **until** $n \geq N$;

Random Scan Gibbs as Metropolis-Hastings

HW

Theorem

The random scan Gibbs sampler is a special case of the Metropolis-Hastings algorithm, in which the proposal is always accepted. In particular, it follows that the stationary distribution of the random scan Gibbs sampler is as desired.

Gibbs Sampling vs. Metropolis-Hastings

- Gibbs sampling emphasizes conditional distributions.
- Metropolis-Hastings emphasizes acceptance probabilities.

Gibbs Sampler for Continuous State Space

In the Gibbs sampler, the target distribution $\boldsymbol{\pi}$ is an m-dimensional joint density

$$\boldsymbol{\pi}(\boldsymbol{x}) = \pi(x_1, \cdots, x_m).$$

A multivariate Markov chain is constructed whose limiting distribution is $\boldsymbol{\pi}$, and which takes values in an m-dimensional space. The algorithm generates elements by iteratively updating each component of an m-dimensional vector conditional on the other $m-1$ components.

Example: Bivariate Standard Normal Distribution

$\rho = \pm 1$,

Joint PDF $f(x,y) = \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{x^2-2\rho xy+y^2}{2(1-\rho^2)}}$,

$-1<\rho<1$,

$-\infty < x, y < \infty$,

$f(x|Y=y) \sim N(\rho y, 1-\rho^2)$

$f(y|X=x) \sim N(\rho x, 1-\rho^2)$

Example: Bivariate Standard Normal Distribution

The Gibbs sampler is implemented to simulate (X, Y) from a bivariate standard normal distribution with correlation ρ.

1. Initialize: $(x_0, y_0) \leftarrow (0, 0)$, $m \leftarrow 1$.
2. Generate x_m from the conditional distribution of X given $Y = y_{m-1}$. That is, simulate from a normal distribution with mean ρy_{m-1} and variance $1 - \rho^2$.
3. Generate y_m from the conditional distribution of Y given $X = x_m$. That is, simulate from a normal distribution with mean ρx_m and variance $1 - \rho^2$.
4. $m \leftarrow m + 1$.
5. Return to Step 2.

$f(x|Y=y_{m-1}) \sim N(\rho y_{m-1}, 1-\rho^2)$

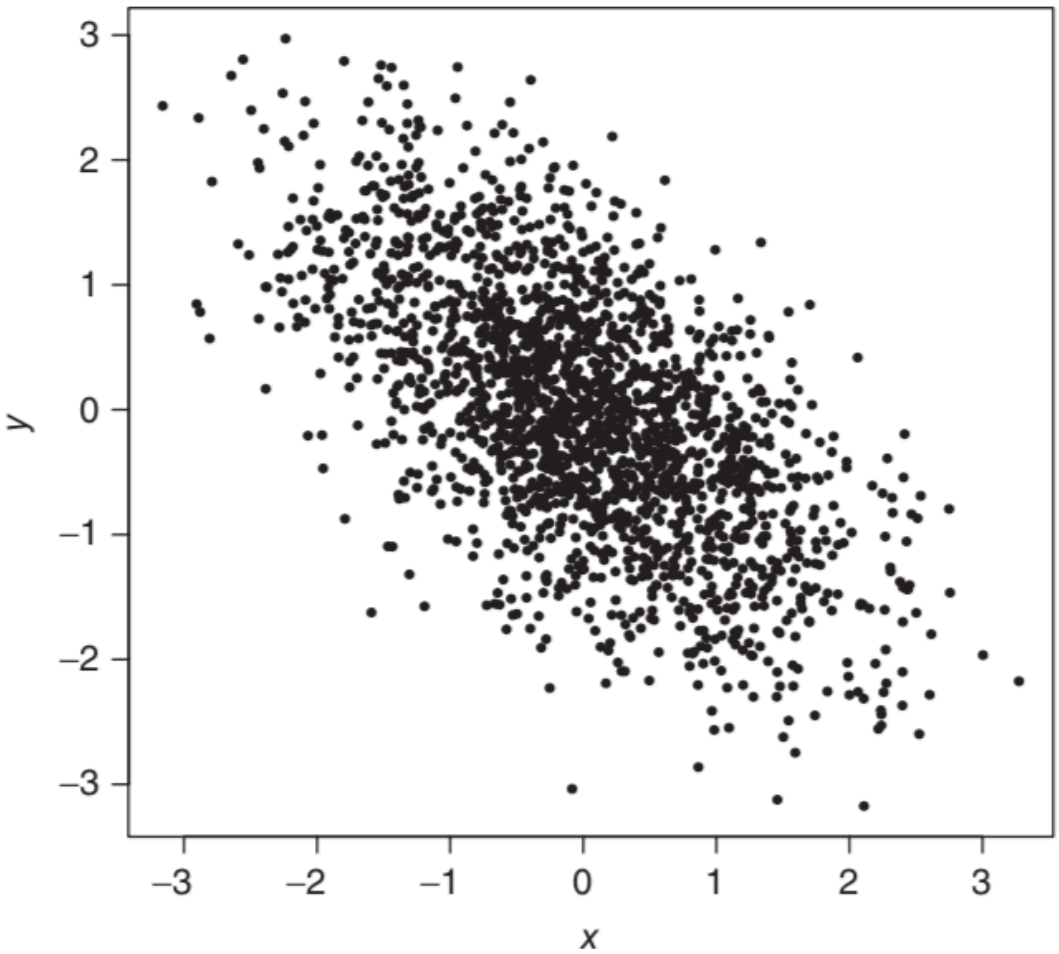
$f(Y|X=x_m) \sim N(\rho x_m, 1-\rho^2)$

$\sim N(\rho x_{m-1}, 1-\rho^2)$

Simulation Results with MCMC

2000

$\rho = -0.6$



Example: Chicken-Egg with Unknown Parameters

A chicken lays N eggs, where $N \sim \text{Pois}(\lambda)$. Each egg hatches with probability p, where p is unknown; we let $p \sim \text{Beta}(a, b)$. The constants λ, a, b are known.

Here's the catch: we don't get to observe N. Instead, we only observe the number of eggs that hatch, X. Describe how to use Gibbs sampling to find $E(p|X = x)$, the posterior mean of p after observing x hatched eggs.

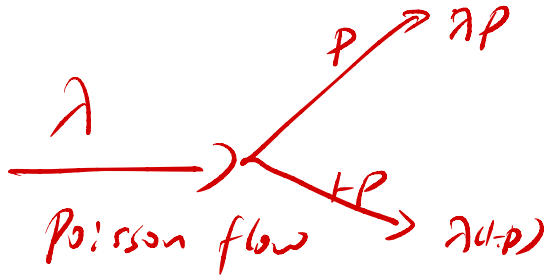
Solution

1°. # of eggs $N \sim Pois(\lambda)$;

# of hatched eggs.

$X | P=p \sim Pois(\lambda p)$.

$N-X | P=p \sim Pois(\lambda(1-p))$.



$f(p|X=x) \propto$ Prob. $(X=x|P=p)$ (likelihood) $\cdot f(p)$ (prior)

$\propto e^{-\lambda p}(\lambda p)^x \cdot p^{a-1}(1-p)^{b-1}$.

we can adopt M-H algorithm to generate samples.

2°. $f_p(p|X=x)$ hard to sample.

$f_{p,N}(p,n|X=x)$ easy to sample.

2.1°. $f(p|N=n, X=x) \sim Beta(x+a, n-x+b)$

$f(n|P=p, X=x) \sim x + Pois(\lambda(1-p))$ shifted poisson.

Solution

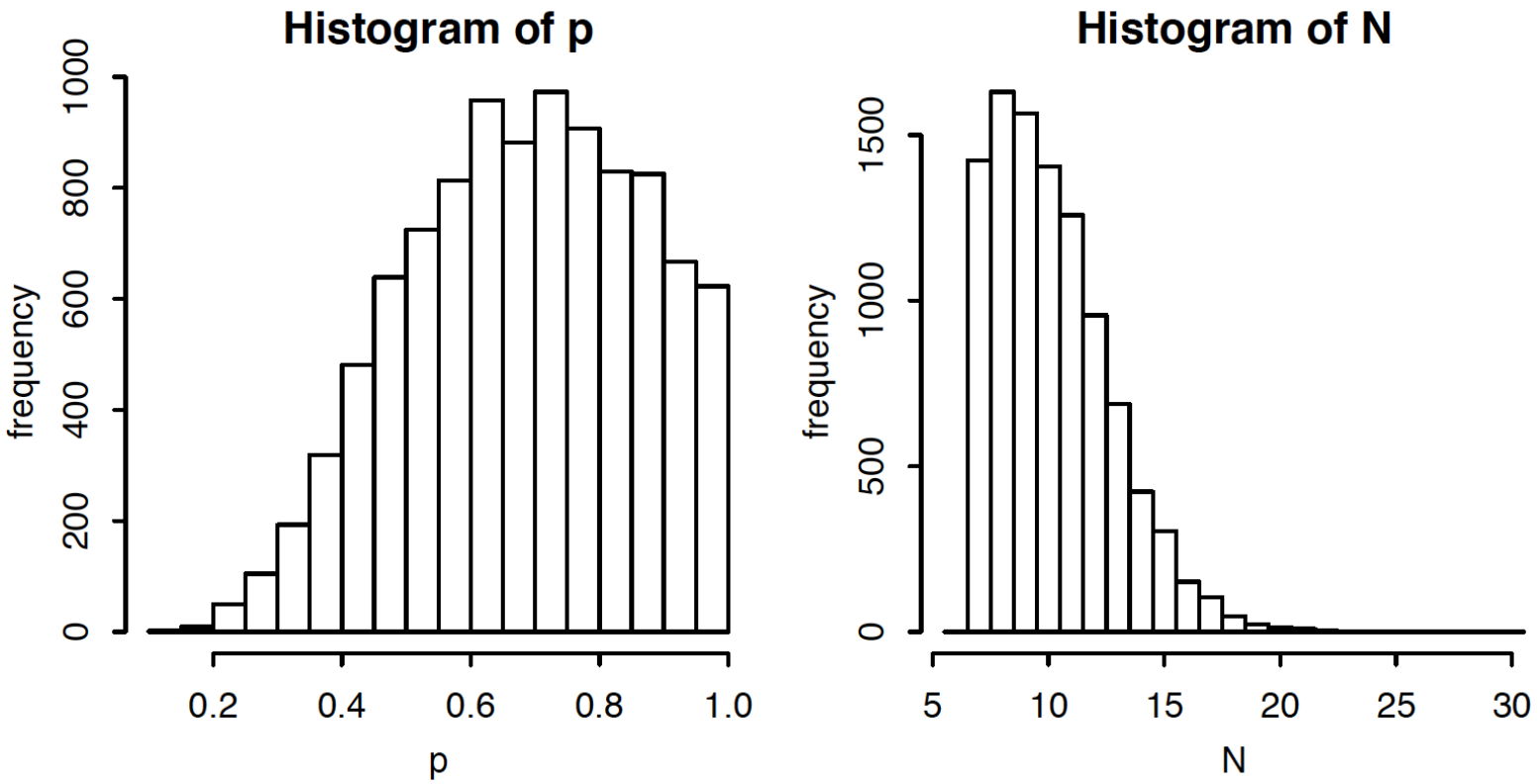
Solution

We make an initial guess for p and N, then iterate the following steps:

1. Conditional on $N = n$ and $X = x$, draw a new guess for p from the $\text{Beta}(x + a, n - x + b)$ distribution.

2. Conditional on p and $X = x$, the number of unhatched eggs is $Y \sim \text{Pois}(\lambda(1 - p))$ by the chicken-egg story, so we can draw Y from the $\text{Pois}(\lambda(1 - p))$ distribution and set the new guess for N to be $N = x + Y$.

Solution



0.68 Sample mean

FIGURE 12.5
Histograms of 10^4 draws from the posterior distributions of p and N, where $\lambda = 10$, $a = 1$, $b = 1$, and we observe $X = 7$.

Example: Three-dimensional Joint Distribution

① PMF. $f(x \mid N=n, P=p) \propto \binom{n}{x} p^x (1-p)^{n-x}$ $\sim Bin(n,p)$

② PDF $f(p \mid X=x, N=n) \propto p^x (1-p)^{n-x}$ $\sim Beta(x+1, n-x+1)$

Random variables X, P and N have joint density

$$\pi(x, p, n) \propto \binom{n}{x} p^x (1-p)^{n-x} \frac{4^n}{n!}$$

for $x = 0, 1, \ldots, n$, $0 < p < 1$, $n = 0, 1, \ldots$. The p variable is continuous; x and n are discrete.

③ PMF $f(n \mid X=x, P=p) \propto \binom{n}{x} (1-p)^{n-x} \frac{4^n}{n!}$

Shifted Poisson. $= x + Z$

$Z \sim Pois(4(1-p))$

Solution

Solution

The Gibbs sampler, with arbitrary initial value, is implemented as follows:

1. Initialize: $(x_0, p_0, n_0) \leftarrow (1, 0.5, 2)$
   $m \leftarrow 1$

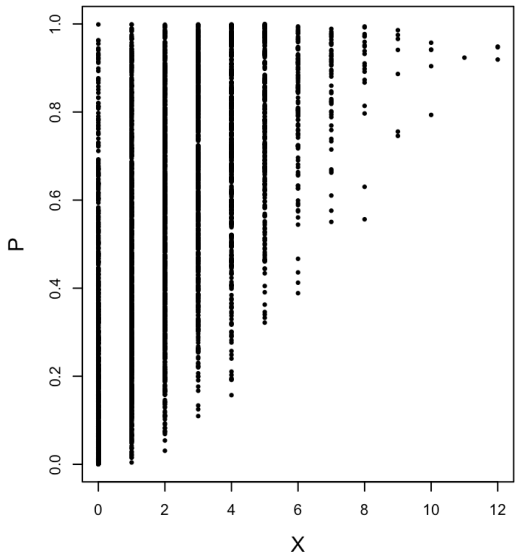
Systematic Scan

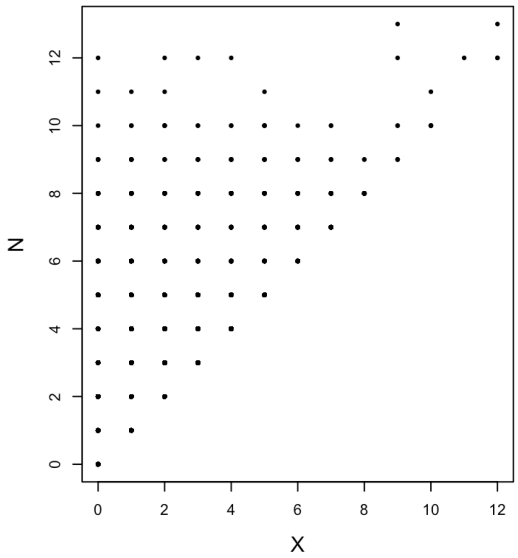
2. Generate x_m from a binomial distribution with parameters n_{m-1} and p_{m-1}.
3. Generate p_m from a beta distribution with parameters $x_m + 1$ and $n_{m-1} - x_m + 1$.
4. Let $n_m = z + x_m$, where z is simulated from a Poisson distribution with parameter $4(1 - p_m)$.
5. $m \leftarrow m + 1$
6. Return to Step 2.

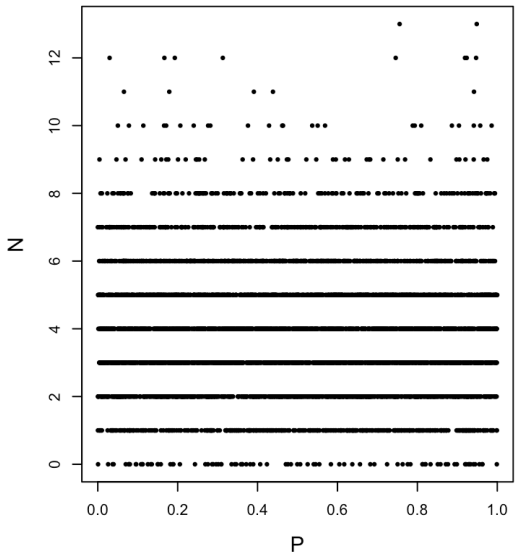
The output of the Gibbs sampler is a sequence of samples

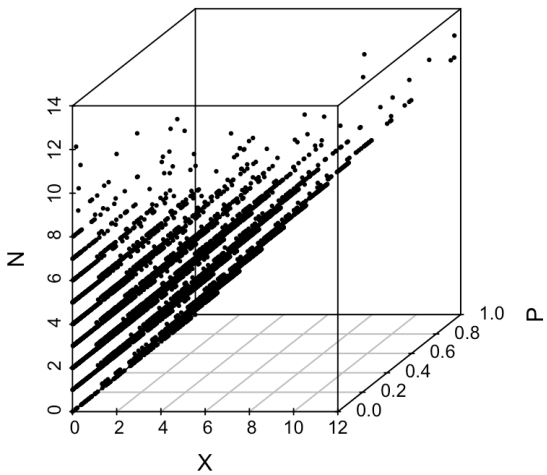
$$(X_0, P_0, N_0), (X_1, P_1, N_1), (X_2, P_2, N_2), \ldots$$

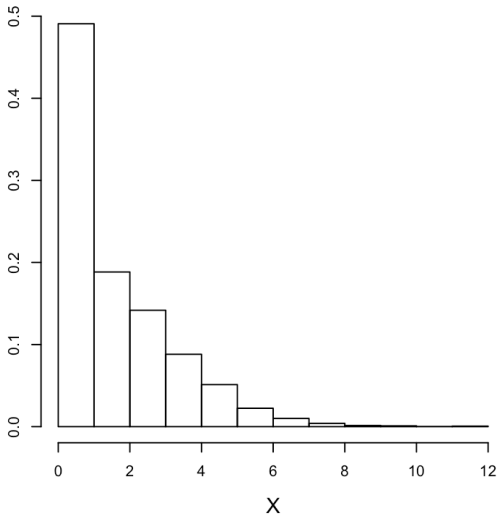
Simulation Results with MCMC

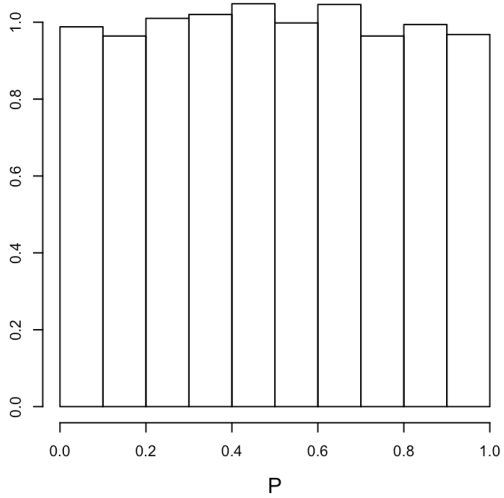












Outline

1 Introduction of MCMC

2 Metropolis–Hastings Algorithm

3 Gibbs Sampler

4 Hamiltonian Monte Carlo Method

5 References

Motivation: Random-Walk Metropolis

Let $Y|\theta \sim \mathcal{N}\left(\theta, \sigma^2\right)$, where σ^2 is known but θ is unknown. Using the Bayesian framework, we treat θ as a random variable, with prior given by $\theta \sim \mathcal{N}\left(\mu, \tau^2\right)$ for some known constants μ and τ^2. That is, we have the two-level model

$$\begin{aligned} \theta &\sim \mathcal{N}\left(\mu, \tau^2\right) \\ Y|\theta &\sim \mathcal{N}\left(\theta, \sigma^2\right) \end{aligned}$$

Describe how to use the Metropolis-Hastings algorithm to find the posterior mean and variance of θ after observing the value of Y.

Solution

1°. $f_{\theta|Y}(\theta|y) \propto f_{Y|\theta}(y|\theta) \cdot f_{\theta}(\theta)$

$\propto e^{-\frac{1}{2\sigma^2}(y-\theta)^2} \cdot e^{-\frac{1}{2\tau^2}(\theta-\mu)^2}$.

Because of Normal-Normal Conjugacy,

$$\theta|Y=y \sim N\left(\frac{\frac{1}{\sigma^2}}{\frac{1}{\sigma^2}+\frac{1}{\tau^2}} y + \frac{\frac{1}{\tau^2}}{\frac{1}{\sigma^2}+\frac{1}{\tau^2}} \mu, \quad \frac{1}{\frac{1}{\sigma^2}+\frac{1}{\tau^2}}\right)$$

↓ posterior mean of $\theta|Y=y$

↓ posterior variance of $\theta|Y=y$

Solution

2^0. M-H.

$\propto e^{-\frac{1}{2\sigma_1^2}(y-\theta)^2} \cdot e^{-\frac{1}{2\tau^2}(\theta-\mu)^2}$

Construct M.C. whose stationary distribution $f_{\theta|Y}(\theta|y)$

Generates $\theta_0, \theta_1, \ldots$

(a) if $\theta_n = x$, propose a new state x' [rwm]

$x' = x + \varepsilon_n \quad \varepsilon_n \sim N(0, d^2)$

$= x + d \cdot N(0,1)$

$\Rightarrow x = x' - d \cdot N(0,1)$

$= x' + d \cdot N(0,1)$.

(b). the acceptance prob.

$\Rightarrow f(x, x') = f(x', x)$

$$\alpha(x, x') = \min\left(\frac{\pi_{x'} f(x', x)}{\pi_x f(x, x')}, 1\right)$$

$$= \min\left(\frac{f_{\theta|Y}(x'|y)}{f_{\theta|Y}(x|y)}, 1\right)$$

Solution

Solution

Simulation Results with MH

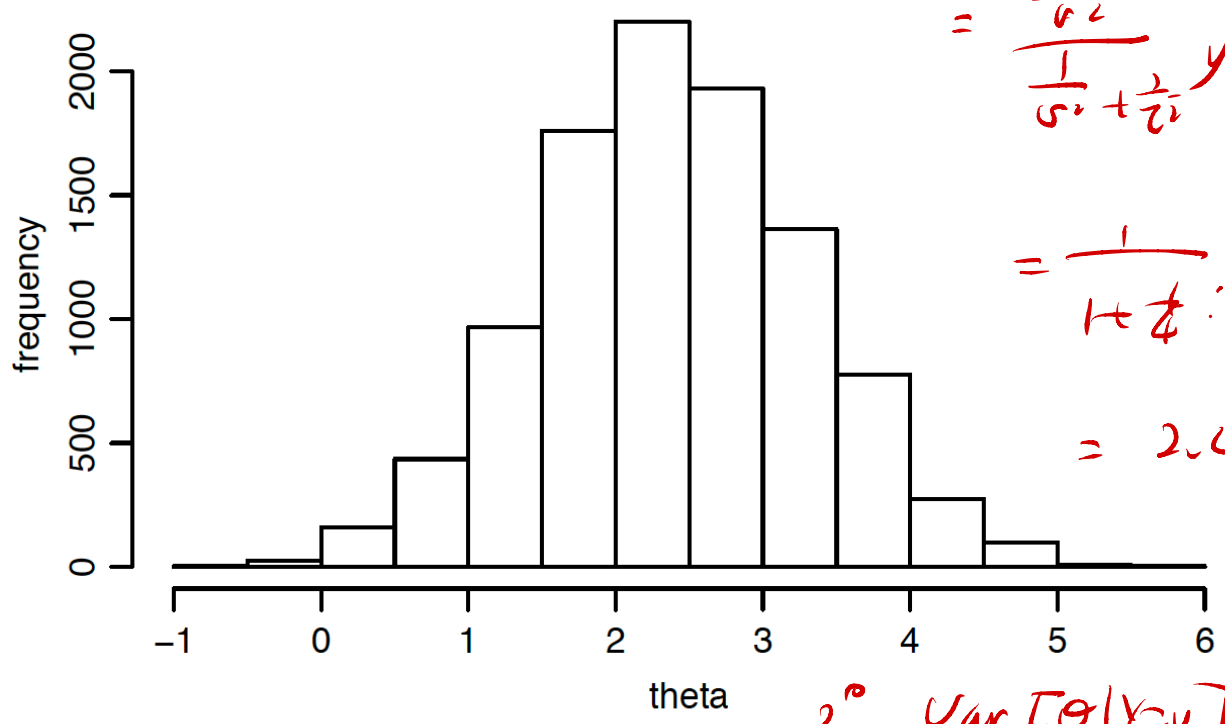


FIGURE 12.2
Histogram of 10^4 draws from the posterior distribution of θ given $Y = 3$, obtained using Metropolis-Hastings with $\mu = 0$, $\sigma^2 = 1$, and $\tau^2 = 4$. The sample mean is 2.4 and the sample variance is 0.8, in agreement with the theoretical values.

Simulation Results with MH

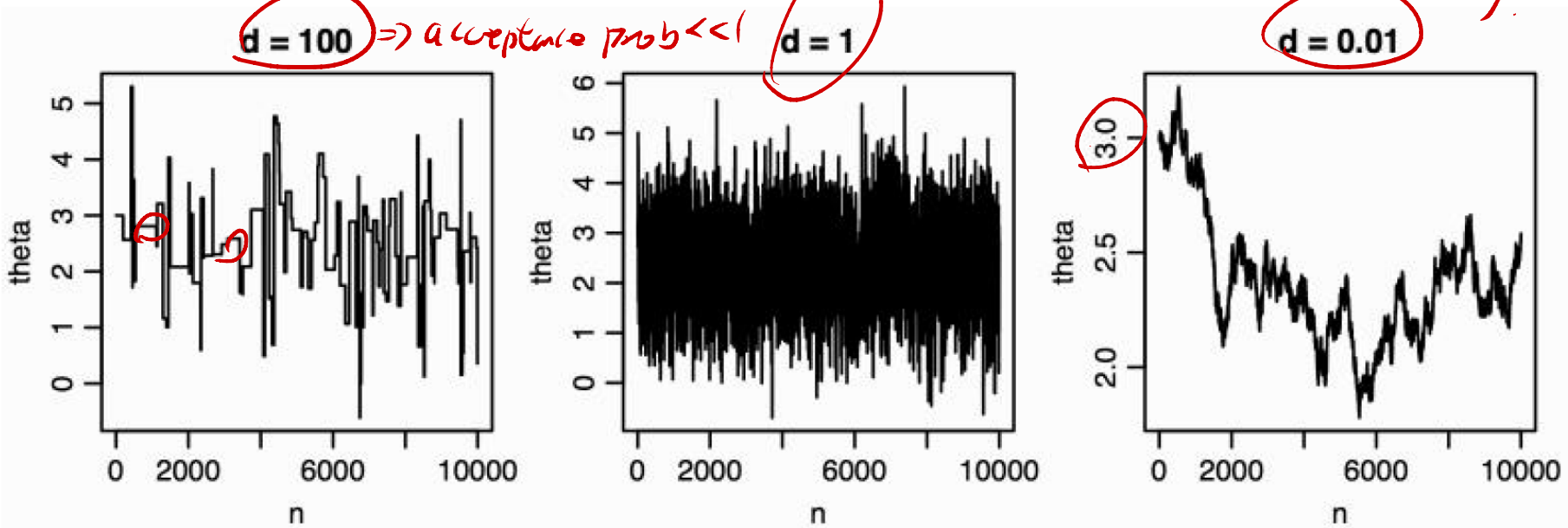


FIGURE 12.3
Trace plots of θ_n as a function of the iteration number n, for $d = 100, 1, 0.01$.

Random Walk Metropolis: RWM

- Continuous state space with target distribution π
- Proposal state:

$$\hat{X}_{n+1} = X_n + \eta \cdot \mathcal{N}(0, \boldsymbol{I})$$

$\boldsymbol{I}$: n-dimension identity matrix.

- One-step transition probability density: $f_{x,y} = f_{y,x}$
- Accept the proposal state with probability

$$a_{X_n, \hat{X}_{n+1}} = \min\left\{1, \frac{\pi(\hat{X}_{n+1})}{\pi(X_n)}\right\}.$$

- Zero-order distribution information with dumb exploration of state space & low acceptance probability in general

Gradient Information

- Explore the state space with gradient information
- Gradient ascent algorithm to find the local maximum of function g:

$$x_{n+1} = x_n + \eta \nabla g(x_n).$$

- Add stochastic noise to avoid stuck in local maximum:

$$x_{n+1} = x_n + \eta \nabla g(x_n) + \sqrt{2\eta} \cdot \mathcal{N}(0, \boldsymbol{I}).$$

- Why $\sqrt{2}$? : Overdamped Langevin Ito diffusion

$$dX_t = \nabla g(X_t)\, dt + \sqrt{2} dB_t$$

with Euler–Maruyama discrete approximation

$$x_{n+1} = x_n + \eta \nabla g(x_n) + \sqrt{2\eta} \cdot \mathcal{N}(0, \boldsymbol{I})$$

Gradient Information

- Now the target distribution is π
- Choice of g : π or $\log(\pi)$?
- The First Choice:

$$x_{n+1} = x_n + \eta \nabla \pi(x_n) + \sqrt{2\eta} \cdot \mathcal{N}(0, \boldsymbol{I}).$$

- The Second Choice:

$$x_{n+1} = x_n + \eta \nabla \log \pi(x_n) + \sqrt{2\eta} \cdot \mathcal{N}(0, \boldsymbol{I}).$$

- Which one is better?

Langevin Monte Carlo: LMC

- Continuous state space with target distribution π
- Proposal state:

$$\hat{X}_{n+1} = X_n + \eta \nabla \log \pi(x_n) + \sqrt{2\eta} \cdot \mathcal{N}(0, \boldsymbol{I})$$

- One-step transition probability density:

$$f_{x,y} \propto \exp\left(-\frac{1}{4\eta}\left(y - x - \eta \nabla \log \pi(x)\right)^2\right).$$

- Accept the proposal state with probability

$$a_{X_n, \hat{x}_{n+1}} = \min\left\{1, \frac{\pi(\hat{X}_{n+1}) f_{\hat{X}_{n+1}, X_n}}{\pi(X_n) f_{X_n, \hat{X}_{n+1}}}\right\}.$$

- Also called Metropolis-adjusted Langevin algorithm (MALA)

Langevin Monte Carlo: LMC

- Usually proposes moves into regions of higher density (π): more likely to be accepted
- Optimal acceptance probability is 0.574 for a limited classes of target distributions
- First-order distribution information with smart exploration of state space & mid acceptance probability in general

Hamiltonian Monte Carlo: HMC

- Random Walk Metropolis (RWM): Zero-order distribution information with dumb exploration of state space & low acceptance probability in general
- Langevin Monte Carlo(LMC): First-order distribution information with smart exploration of state space & mid acceptance probability in general
- Can we find MCMC methods with smart exploration of state space & high acceptance probability in general?
- Yes, We Can!

Hamiltonian Dynamics

- Classical mechanics (or Newtonian mechanics):

$$\boldsymbol{F} = m\boldsymbol{a} = m\frac{d^2\boldsymbol{x}_t}{dt^2}.$$

- Lagrangian mechanics with Lagrangian:

$$L(\boldsymbol{x}_t, \boldsymbol{x}_t', t) = V - U = \text{Kinetic Energy} - \text{Potential Energy}.$$

- Tautochrone curve problem motivated Euler-Lagrange equation and the calculus of variations
- Hamiltonian mechanics(also called Hamiltonian dynamics): reformulation of Lagrangian mechanics with momenta

Hamiltonian Dynamics

- d-dimensional space
- $\boldsymbol{x}$: position vector of the moving object
- $U(\boldsymbol{x})$: potential energy
- $\boldsymbol{\omega}$: momentum vector of the moving object
- $V(\boldsymbol{\omega})$: Kinetic Energy
- $H(\boldsymbol{x}, \boldsymbol{\omega}) = U(\boldsymbol{x}) + V(\boldsymbol{\omega})$: Hamiltonian(energy)
- $\{(\boldsymbol{x}, \boldsymbol{\omega})\}$: phase space(coordinate system that is defined in terms of position and momentum)
- Hamiltonian equations: $j = 1, \ldots, d$

$$\frac{dx_j}{dt} = \frac{\partial H}{\partial \omega_j}$$
$$\frac{d\omega_j}{dt} = -\frac{\partial H}{\partial x_j}.$$

$$\frac{dH(x,\omega)}{dt} = \sum_{j=1}^{d} \left\{ \frac{\partial H}{\partial x_j}\frac{dx_j}{dt} + \frac{\partial H}{\partial \omega_j}\frac{d\omega_j}{dt} \right\}$$
$$= \sum_{j=1}^{d} \left\{ \frac{\partial H}{\partial x_j}\cdot\frac{\partial H}{\partial \omega_j} + \frac{\partial H}{\partial \omega_j}\cdot\left(-\frac{\partial H}{\partial x_j}\right) \right\}$$
$$= 0$$
$$\Rightarrow H(x,\omega) = \text{const}$$

Hamiltonian Dynamics: Numerical Solution

- No analytical solution for Hamiltonian equations
- Approximation with Taylor expansion: $\forall j = 1, \ldots, d$

$$x_j(t+\delta) \approx x_j(t) + \delta \frac{dx_j}{dt} = x_j(t) + \delta \frac{\partial H(\boldsymbol{x}_t, \boldsymbol{\omega}_t)}{\partial \omega_j} = x_j(t) + \delta \frac{\partial V(\boldsymbol{\omega}_t)}{\partial \omega_j}$$

$$\omega_j(t+\delta) \approx \omega_j(t) + \delta \frac{d\omega_j}{dt} = \omega_j(t) - \delta \frac{\partial H(\boldsymbol{x}_t, \boldsymbol{\omega}_t)}{\partial x_j} = \omega_j(t) - \delta \frac{\partial U(\boldsymbol{x}_t)}{\partial x_j}$$

- Three methods: Euler's Method, Modified Euler's Method, The Leapfrog Method

Numerical Solution I: Euler's Method

x_j, ω_j both updated.

instability

$$\omega_j(t+\delta) = \omega_j(t) - \delta \frac{\partial U(\boldsymbol{x}_t)}{\partial x_j}$$

$$x_j(t+\delta) = x_j(t) + \delta \frac{\partial V(\boldsymbol{\omega}_t)}{\partial \omega_j}.$$

Numerical Solution II: Modified Euler's Method

$$\omega_j(t+\delta) = \omega_j(t) - \delta \frac{\partial U(\boldsymbol{x}_t)}{\partial x_j}$$

$$x_j(t+\delta) = x_j(t) + \delta \frac{\partial V(\boldsymbol{\omega}_{t+\delta})}{\partial \omega_j}.$$

Alternate updated

stable

Numerical Solution III: The Leapfrog Method

half step

$$\omega_j\left(t+\frac{\delta}{2}\right) = \omega_j(t) - \frac{\delta}{2}\cdot\frac{\partial U(\boldsymbol{x}_t)}{\partial x_j}$$

one-step

$$x_j(t+\delta) = x_j(t) + \delta\cdot\frac{\partial V\left(\boldsymbol{\omega}_{t+\frac{\delta}{2}}\right)}{\partial \omega_j}$$

$$\omega_j(t+\delta) = \omega_j\left(t+\frac{\delta}{2}\right) - \frac{\delta}{2}\cdot\frac{\partial U(\boldsymbol{x}_{t+\delta})}{\partial x_j}$$

half step

Example

- $d = 1$ initial position $x_0 = 0$, initial momentum $\omega_0 = 1$
- $H(x, \omega) = U(x) + V(\omega) = \frac{x^2}{2} + \frac{\omega^2}{2}$
- Phase space:

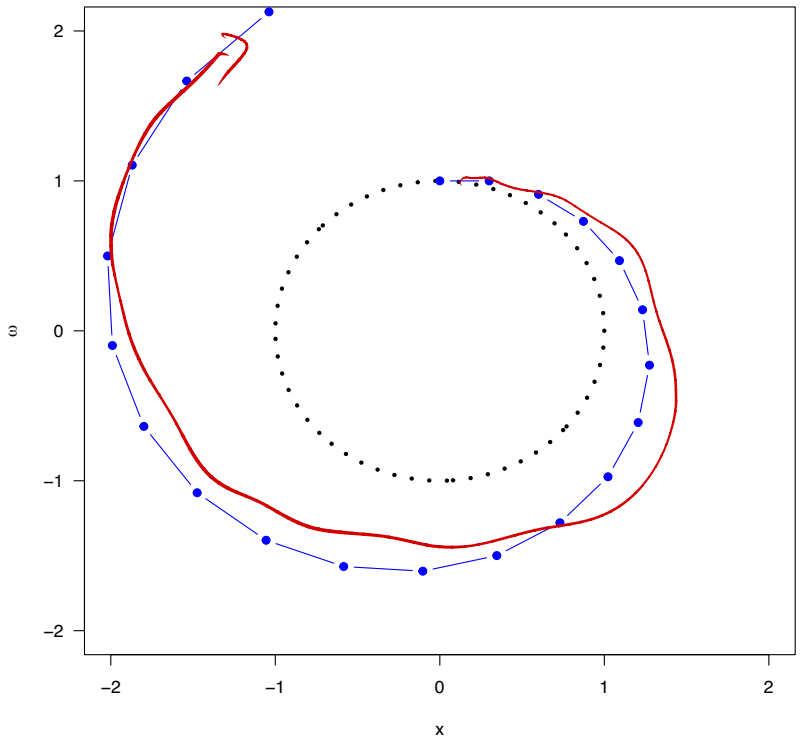
$$H(x_t, \omega_t) = \frac{x_t^2}{2} + \frac{\omega_t^2}{2} = H(x_0, \omega_0) = \frac{x_0^2}{2} + \frac{\omega_0^2}{2} = \frac{1}{2}.$$

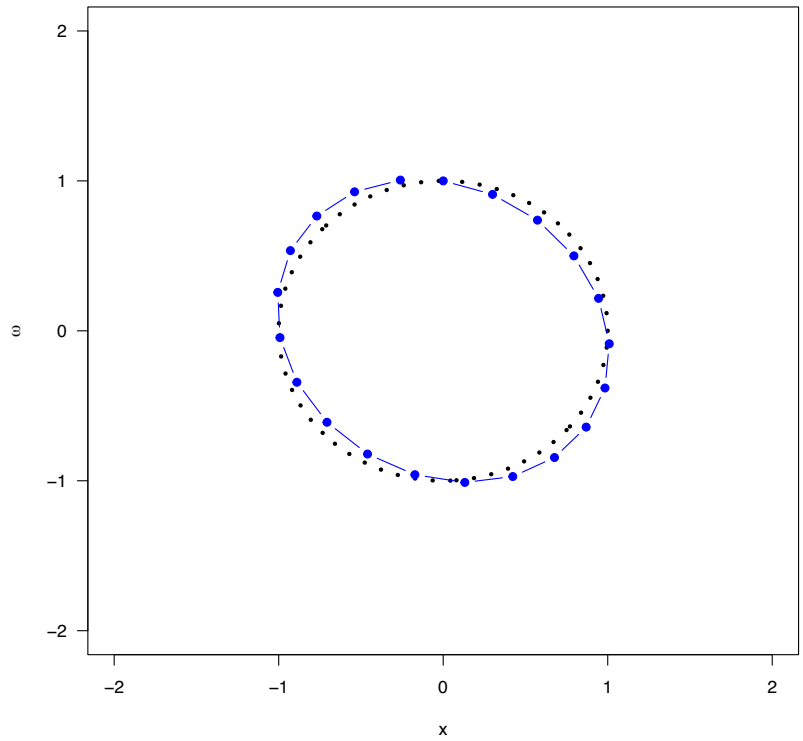
- Equivalent expression:

$$x_t^2 + \omega_t^2 = 1, \forall t \geq 0$$

Example

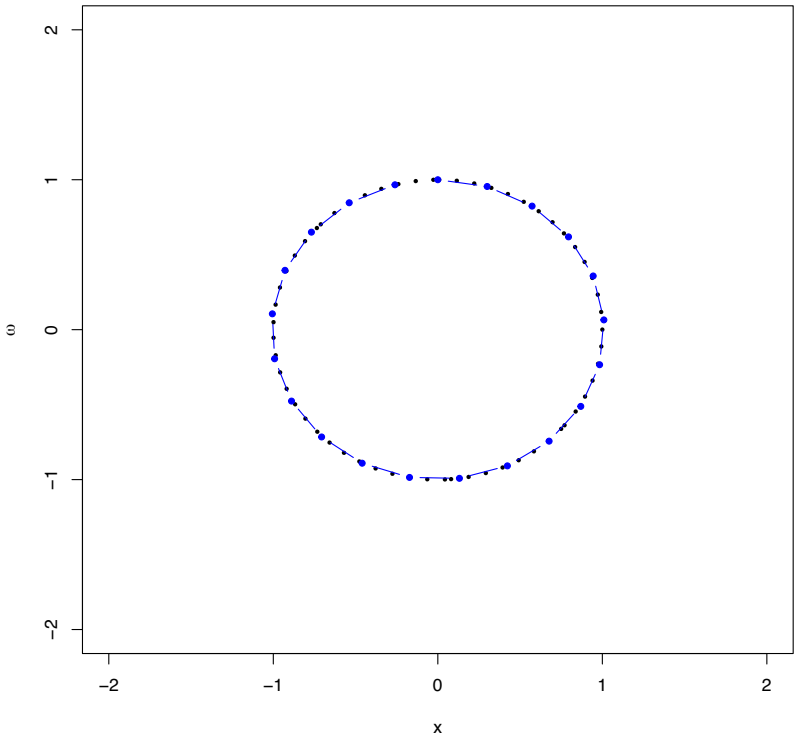
- Step size $\delta = 0.3$ with 20 steps
- LHS is the result with Euler's Method
- RHS is the result with Modified Euler's Method

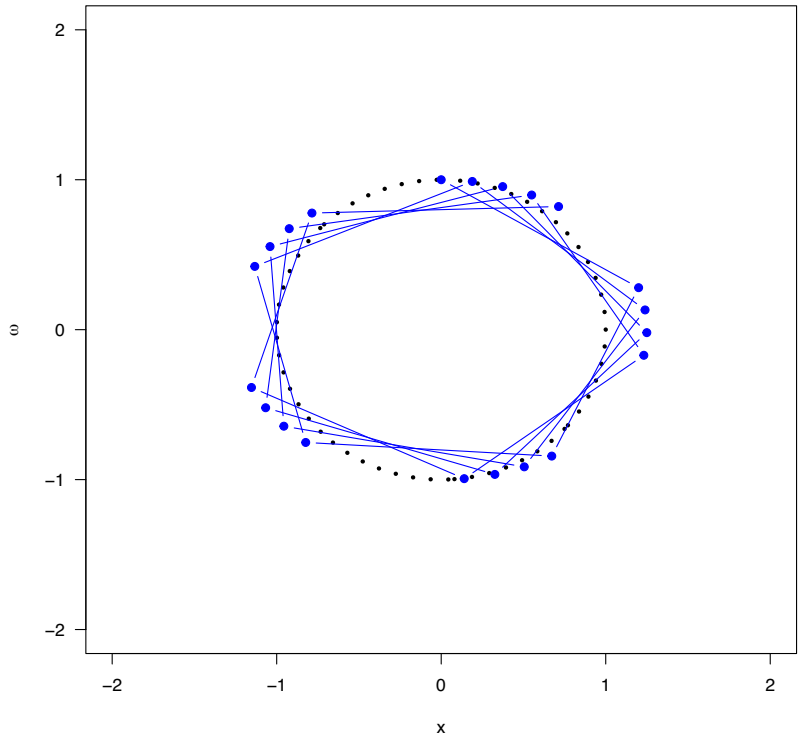




Example

- Both adopt The Leapfrog Method
- LHS is the result with step size $\delta = 0.3$ & 20 steps
- RHS is the result with step size $\delta = 1.2$ & 20 steps





Hamiltonian Monte Carlo: HMC

- Main variable: position $\boldsymbol{x} \in \mathbb{R}^d$ of the moving object
- Target distribution $\pi(\boldsymbol{x})$ is the distribution of the position
- Auxiliary variable: momentum $\boldsymbol{\omega} \in \mathbb{R}^d$ of the moving object
- State of the Markov process: $(\boldsymbol{x}, \boldsymbol{\omega})$
- State space: phase space of corresponding Hamiltonian Dynamics
- Stationary distribution (joint pdf) over the state space:

$$p(\boldsymbol{x}, \boldsymbol{\omega}) \propto e^{-H(\boldsymbol{x},\boldsymbol{\omega})} = e^{-U(\boldsymbol{x})-V(\boldsymbol{\omega})} = e^{-U(\boldsymbol{x})} \cdot e^{-V(\boldsymbol{\omega})}.$$

Hamiltonian Monte Carlo: HMC

- Stationary distribution (joint pdf) over the state space:

$$p(\boldsymbol{x}, \boldsymbol{\omega}) \propto e^{-H(\boldsymbol{x},\boldsymbol{\omega})} = e^{-U(\boldsymbol{x})-V(\boldsymbol{\omega})} = e^{-U(\boldsymbol{x})} \cdot e^{-V(\boldsymbol{\omega})} = \pi(\boldsymbol{x}) \cdot \pi(\boldsymbol{\omega}).$$

- Set $e^{-U(\boldsymbol{x})} = \pi(\boldsymbol{x})$, then

$$U(\boldsymbol{x}) = -\log(\pi(\boldsymbol{x})).$$

- Set $e^{-V(\boldsymbol{\omega})} = \pi(\boldsymbol{\omega})$, usually choose multivariate Normal distribution:

$$\pi(\boldsymbol{\omega}) \propto e^{-\frac{1}{2}\boldsymbol{\omega}^T \Sigma^{-1} \boldsymbol{\omega}} \sim \mathcal{N}(0, \Sigma)$$

where

$$\Sigma = \mathrm{diag}(m_1, \ldots, m_d).$$

Mass Matrix

then

$$V(\boldsymbol{\omega}) = \sum_{j=1}^{d} \frac{\omega_j^2}{2m_j}, \forall m_j > 0.$$

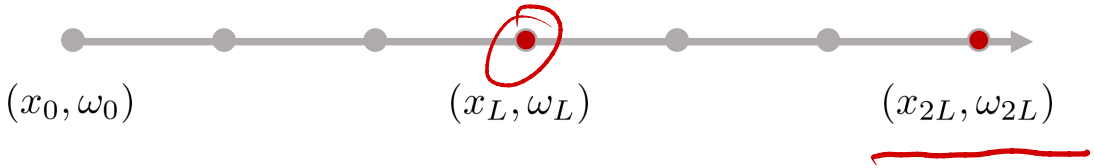
One-Round Hamiltonian Monte Carlo

- Start with a given initial position $\boldsymbol{x}_0$
- Set the initial momentum $\boldsymbol{\omega}_0$ as one sample from $\mathcal{N}(0, \boldsymbol{\Sigma})$.
- Apply the leapfrog method with initial state $(\boldsymbol{x}_0, \boldsymbol{\omega}_0)$ with step-size δ and step number L; then record state $(\boldsymbol{x}_L, \boldsymbol{\omega}_L)$
- Reverse the direction of momentum and obtain the state $(\boldsymbol{x}_L, -\boldsymbol{\omega}_L)$.
- Set the state $(\boldsymbol{x}_L, -\boldsymbol{\omega}_L)$ as the proposal state.
- Accept the proposal state with probability

$$
\begin{aligned}
a_{(\boldsymbol{x}_0,\boldsymbol{\omega}_0),(\boldsymbol{x}_L,-\boldsymbol{\omega}_L)} &= \min\left\{1, \frac{\exp\left(-H(\boldsymbol{x}_L, -\boldsymbol{\omega}_L)\right)}{\exp\left(-H(\boldsymbol{x}_0, \boldsymbol{\omega}_0)\right)}\right\} \\
&= \min\left\{1, \frac{\exp\left(-U(\boldsymbol{x}_L) - V(-\boldsymbol{\omega}_L)\right)}{\exp\left(-U(\boldsymbol{x}_0) - V(\boldsymbol{\omega}_0)\right)}\right\}.
\end{aligned}
$$

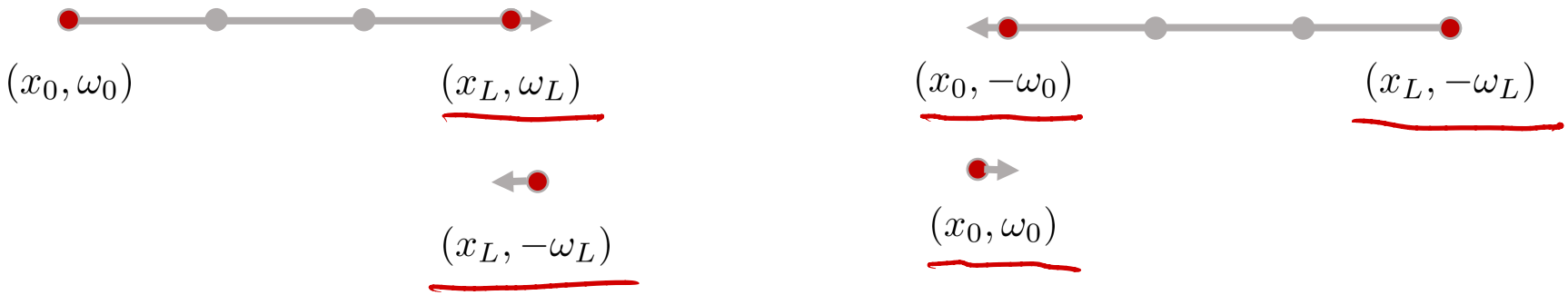
Why Reverse the Direction of Momentum?

$$f((x_L, \omega_L)|(x_0, \omega_0)) > 0$$



$$f((x_0, \omega_0)|(x_L, \omega_L)) = 0$$

Why Reverse the Direction of Momentum?



$$f((x_L, -\omega_L)|(x_0, \omega_0)) = f((x_0, \omega_0)|(x_L, -\omega_L)) > 0$$

Acceptance Probability is Close to 1

$$
\begin{aligned}
a_{(\boldsymbol{x}_0,\boldsymbol{\omega}_0),(\boldsymbol{x}_L,-\boldsymbol{\omega}_L)} &= \min\left\{1, \frac{p(\boldsymbol{x}_L,-\boldsymbol{\omega}_L)f((\boldsymbol{x}_0,\boldsymbol{\omega}_0)|(\boldsymbol{x}_L,-\boldsymbol{\omega}_L))}{p(\boldsymbol{x}_0,\boldsymbol{\omega}_0)f((\boldsymbol{x}_L,-\boldsymbol{\omega}_L)|(\boldsymbol{x}_0,\boldsymbol{\omega}_0))}\right\} \\
&= \min\left\{1, \frac{p(\boldsymbol{x}_L,-\boldsymbol{\omega}_L)}{p(\boldsymbol{x}_0,\boldsymbol{\omega}_0)}\right\} \\
&= \min\left\{1, \frac{\exp\left(-H(\boldsymbol{x}_L,-\boldsymbol{\omega}_L)\right)}{\exp\left(-H(\boldsymbol{x}_0,\boldsymbol{\omega}_0)\right)}\right\} \\
&= \min\left\{1, \frac{\exp\left(-U(\boldsymbol{x}_L)-V(-\boldsymbol{\omega}_L)\right)}{\exp\left(-U(\boldsymbol{x}_0)-V(\boldsymbol{\omega}_0)\right)}\right\}.
\end{aligned}
$$

Example I

- Target distribution(PDF):

$$f(x) = \frac{8}{3\pi\sqrt{5}}\left(1+\frac{1}{5}x^2\right)^{-3}, -\infty < x < \infty.$$

$g(x)$

$f(x) \propto (1+\frac{1}{5}x^2)^{-3}$

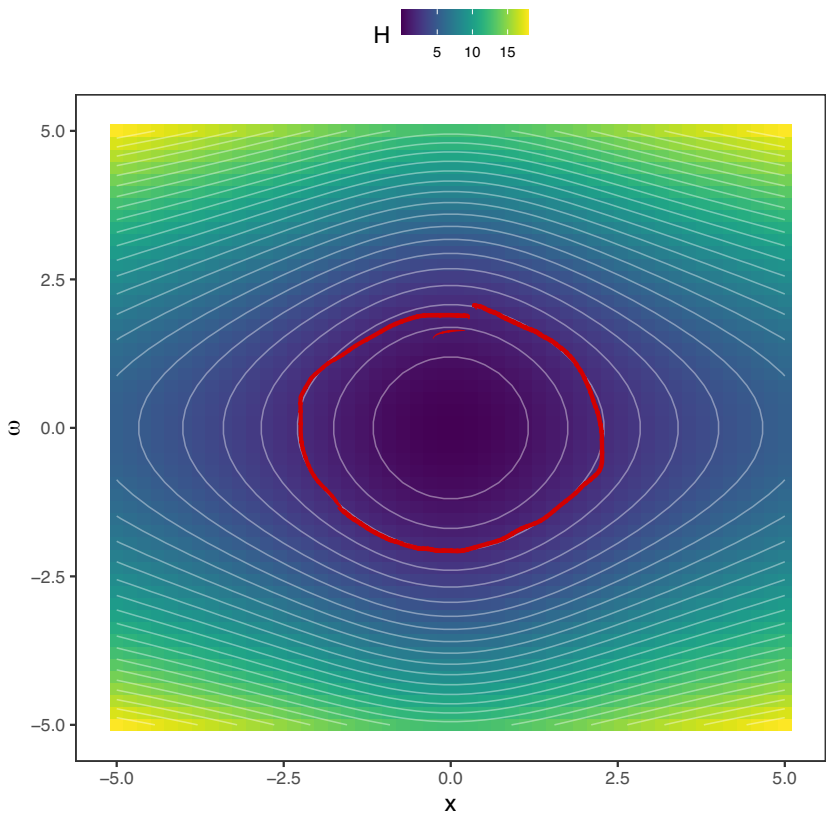
$U(x) = -\log g(x)$

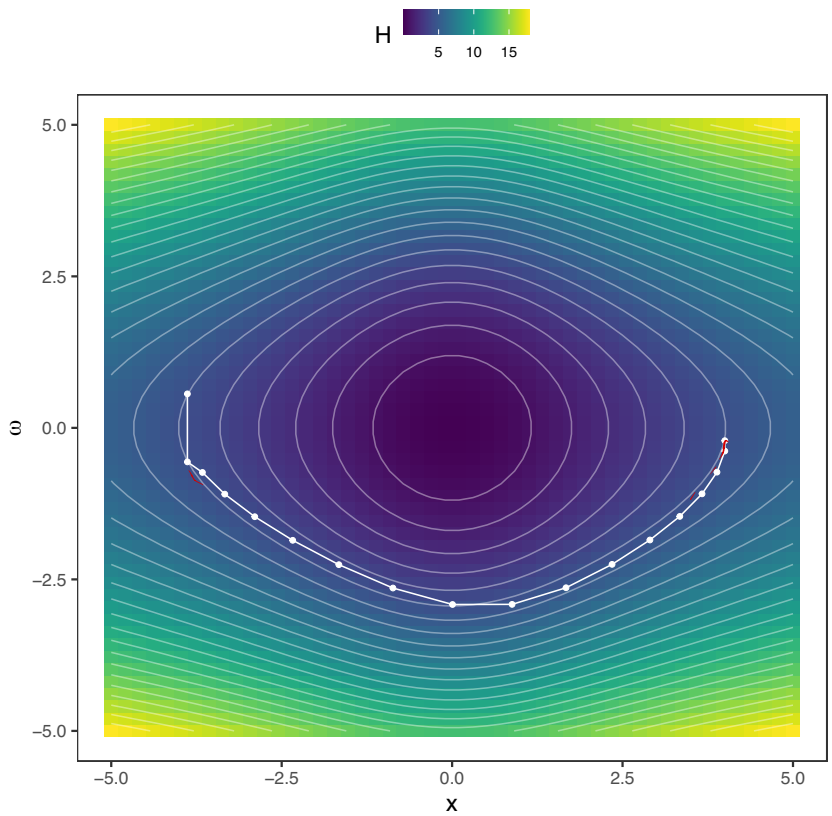
$= 3\log(1+\frac{1}{5}x^2)$

$V(\omega) = \frac{1}{2}\omega^2, \quad \omega \sim N(0,1)$

Example I

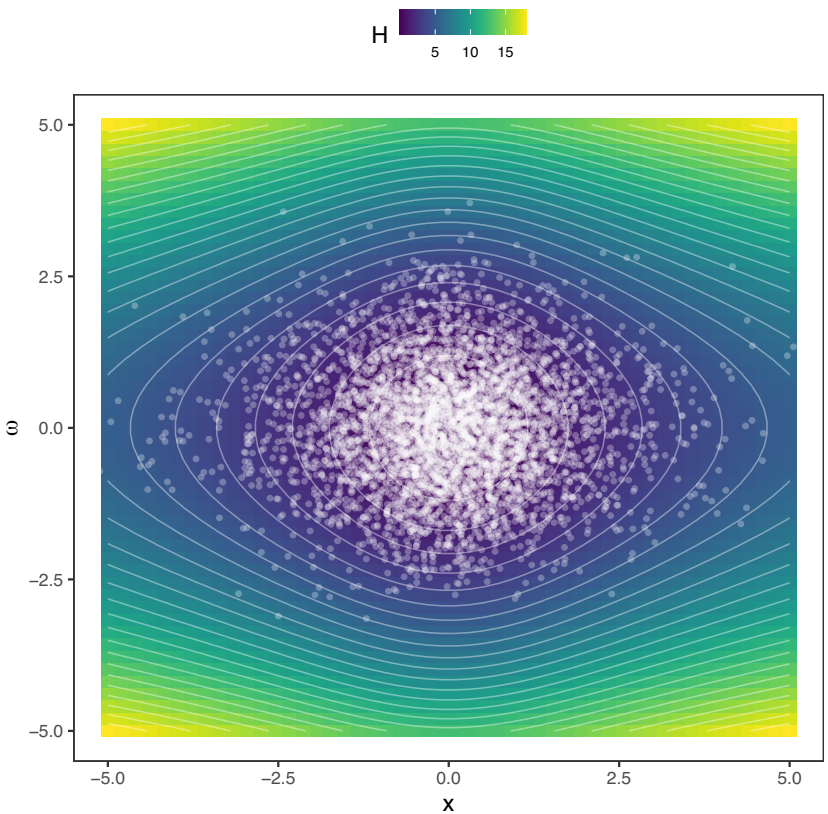
$\delta = 0.3, \quad L = 15$

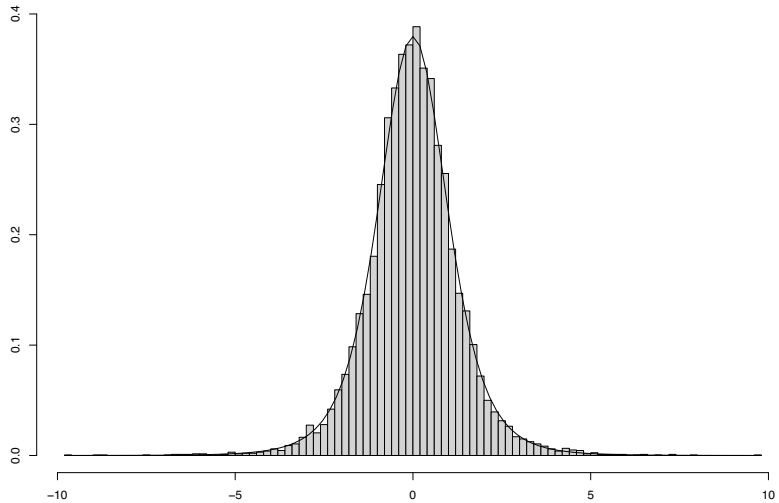




Example I

T = 1000





Example II: Gaussian Mixture Distribution

$f(x) \propto \underbrace{0.4\, e^{-\frac{1}{2}(x-2)^2} + 0.6 \cdot e^{-\frac{1}{2}(x+2)^2}}_{g(x)}$

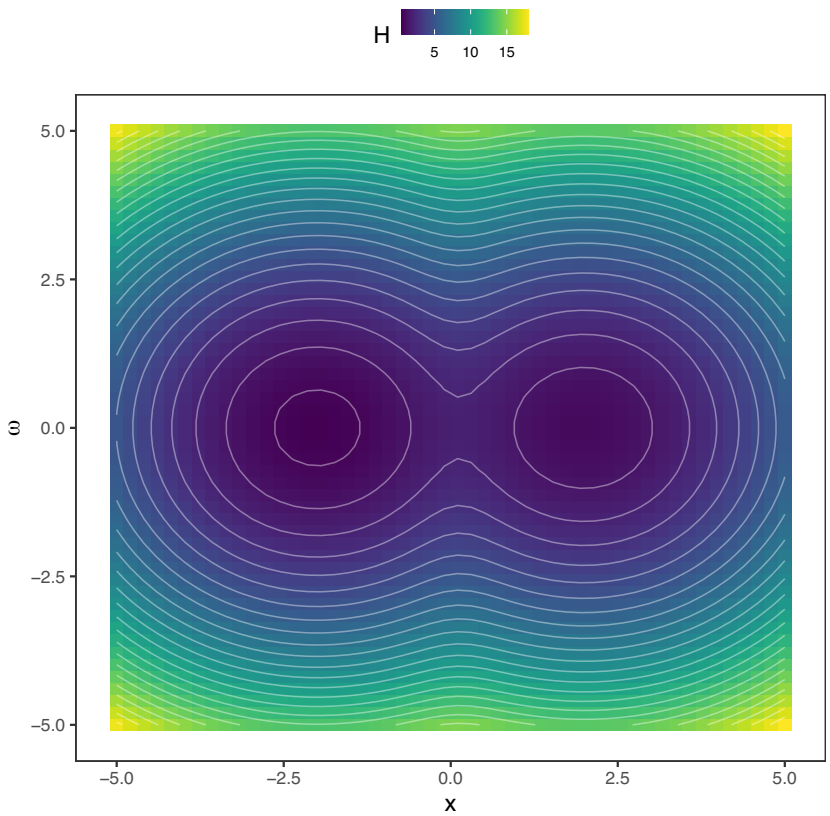
- Target distribution(PDF):

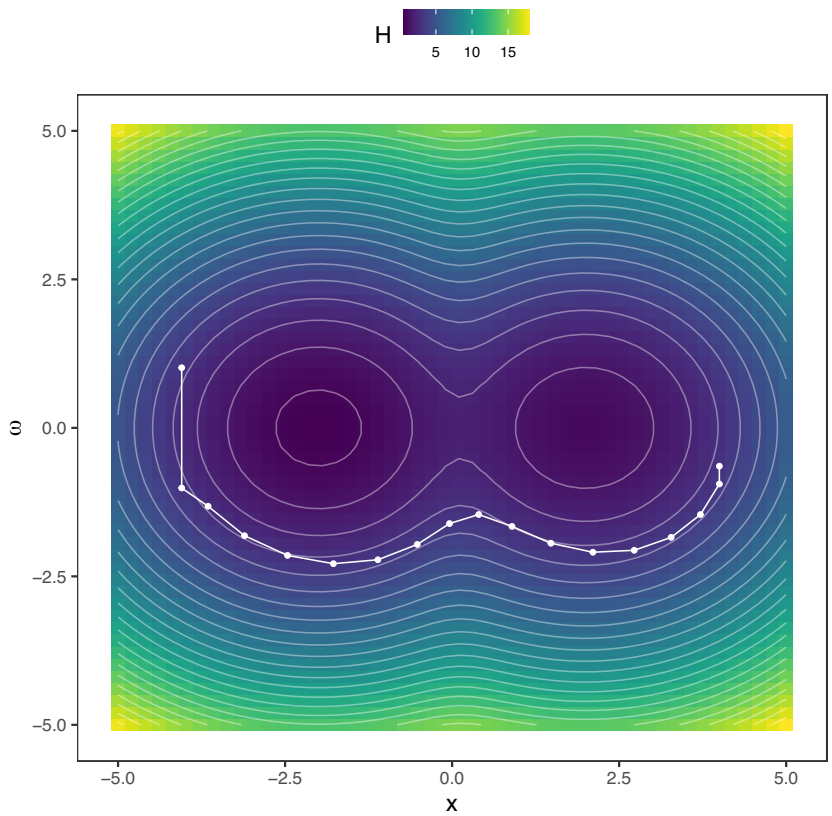
$U(x) = -\log g(x) = -\log(\quad)$

$$f(x) = 0.4 \cdot \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(x-2)^2} + 0.6 \cdot \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(x+2)^2}, \quad -\infty < x < \infty.$$

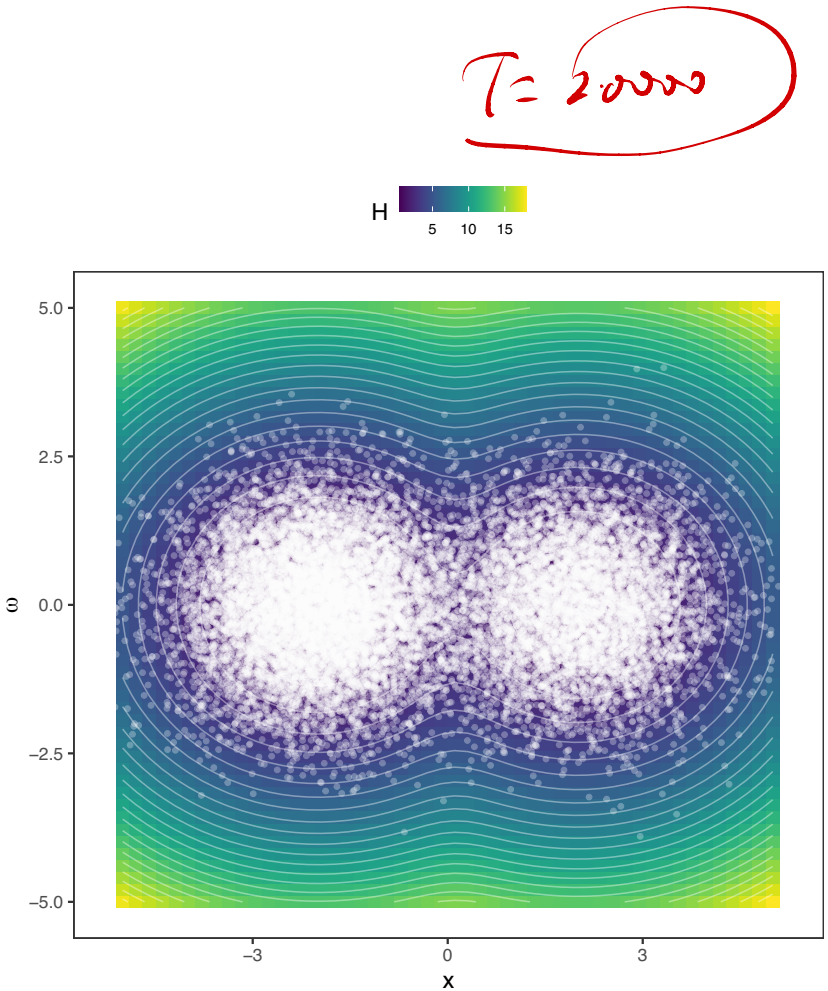
$U(\omega) = \frac{1}{2}\omega^2, \quad \omega \in N(0,1)$

Example II


H
5
10
15
5.0
2.5
0.0
−2.5
−5.0
ω
−5.0
−2.5
0.0
2.5
5.0
x


H
5
10
15
5.0
2.5
0.0
−2.5
−5.0
ω
−5.0
−2.5
0.0
2.5
5.0
x

Example II

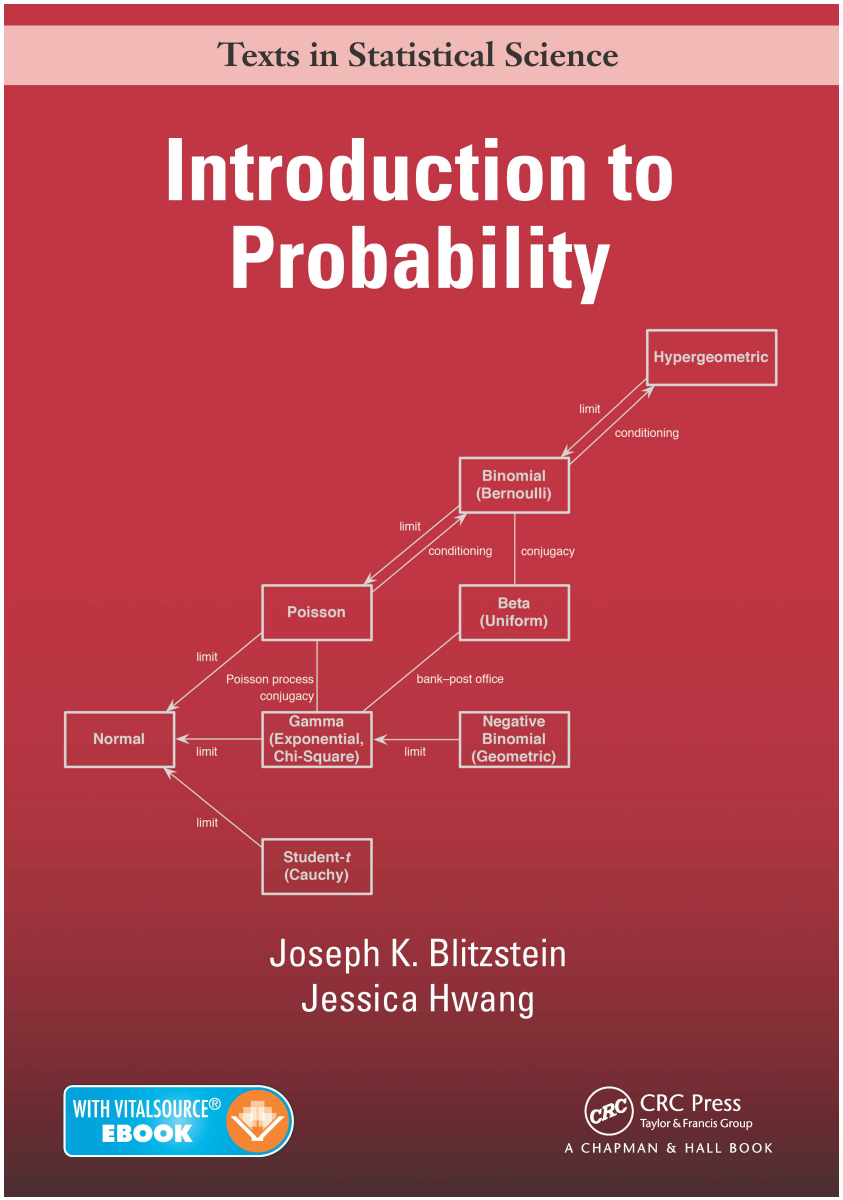

T= 20000
H
5
10
15
5.0
2.5
0.0
−2.5
−5.0
ω
−3
0
3
x


0.25
0.20
0.15
0.10
0.05
0.00
−6
−4
−2
0
2
4
6

Outline

1. Introduction of MCMC
2. Metropolis–Hastings Algorithm
3. Gibbs Sampler
4. Hamiltonian Monte Carlo Method
5. References

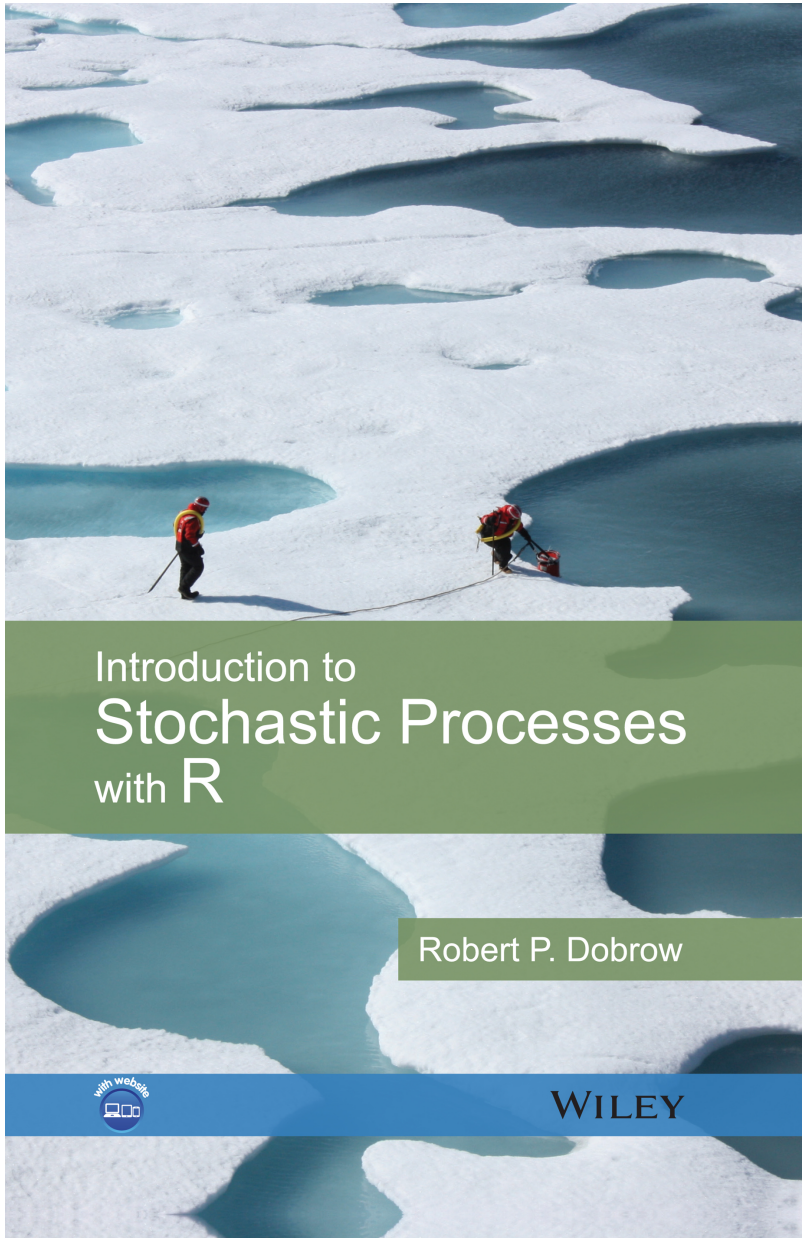
BH



BH

- Introduction to Probability
- Chapman & Hall/CRC, 2014.
- Chapman & Hall/CRC, 2019.
- Chapter 12

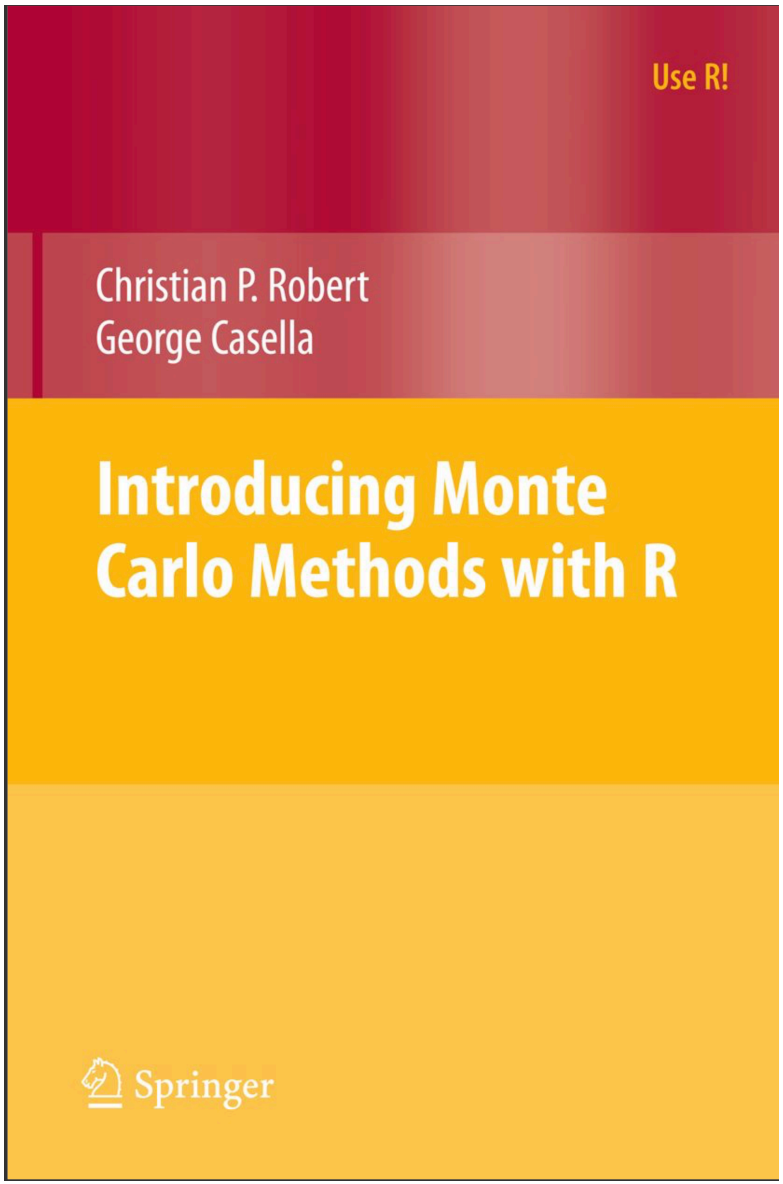
SRR



SPR

- Introduction to Stochastic Processes with R
- John Wiley & Son, 2016.
- Chapter 5

RC



RC

- Introducing Monte Carlo Methods with R
- Springer, 2010.
- All chapters including Chapter 8 (when to stop MCMC algorithm)

Others

- Betancourt, Michael (2018). "A Conceptual Introduction to Hamiltonian Monte Carlo". arXiv:1701.02434
- Neal, Radford M (2011). "MCMC Using Hamiltonian Dynamics"