STAT 576 Bayesian Analysis

Lecture 8: Markov Chain Simulation

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Backgrounds on Markov Chain

Let $\{X_t\}$ be a sequence of random variables. We say $\{X_t\}$ is a **Markov chain** if

$$P(X_{t+1} = x_{t+1} | X_t = x_t, X_{t-1} = x_{t-1}, \ldots, X_0 = x_0) = P(X_{t+1} = x_{t+1} | X_t = x_t).$$

In other words, the future state of the chain depends only on the current state, not on the past states.

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Remarks:

- If $t \in \mathbb{Z}^+$, then $\{X_t\}$ is a **discrete-time** Markov chain.
- If $t \in \mathbb{R}^+$, then $\{X_t\}$ is a **continuous-time** Markov chain.

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- If $t \in \mathbb{Z}^+$, then $\{X_t\}$ is a **discrete-time** Markov chain.
- If $t \in \mathbb{R}^+$, then $\{X_t\}$ is a **continuous-time** Markov chain.
- For discrete-time Markov chain, we can define the **transition probability** $P_{ij,t} = P(X_{t+1} = j | X_t = i)$.
- For continuous-time Markov chain, we can define the **transition rate** $q_{ij,t} = \lim_{s \downarrow t} \frac{P(X_s = j | X_t = i) - \delta_{ij}}{s - t}$.

For now, we will focus on discrete-time Markov chain.

Backgrounds on Markov Chain

For discrete-time Markov chain with transition probability

$$P_{ij,t} = P(X_{t+1} = j | X_t = i),$$

- A Markov chain is **(time-)homogeneous** if the transition probabilities do not depend on t. Otherwise it is **(time-)inhomogeneous**.

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- A Markov chain is **(time-)homogeneous** if the transition probabilities do not depend on t. Otherwise it is **(time-)inhomogeneous**.
- The **state space** of the chain is the set of all possible values of X_t.
- For a finite state space, we represent the transition probabilities in a matrix form, known as **the transition matrix**.
- For a measurable state space, we call it a **Markov chain on a measurable state space**. And we define the **transition kernel**

$$P(x, A) = P(X_{t+1} \in A | X_t = x), \quad x \in \mathcal{X}, A \in \mathcal{B}(\mathcal{X}).$$

For now, we focus on homogenoeous Markov chains with finite state space.

Properties of Markov Chain

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- A Markov chain is **irreducible** if any two states are communicating.
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- The **period** of a state i is the greatest common divisor of all $n \geq 1$ such that $P(X_n = i | X_0 = i) > 0$. If the period is 1, then the state is **aperiodic**.
- A state i is **transient** if there is a non-zero probability that the chain will never return to i. Otherwise, it is **recurrent**.
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- Periodicity, transience, recurrence and postive-recurrence are class properties.

Stationary Distribution of a Markov Chain

- A distribution π on the state space is **stationary** for a Markov chain with transition matrix P if

$$\pi = \pi P.$$

That is $\pi(i) = \sum_j \pi(j) P_{ji}$ for all i.

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- **Covergence theorem**:
If the chain is irreducible and aperiodic with stationary π, then there exist constants $0 < \alpha < 1$ and $C > 0$ such that
$$\max_x \ \|P^t(x, \cdot) - \pi\|_{TV} \leq C\alpha^t.$$

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  $$\frac{V_i(n)}{n} \to \pi(i), \quad \text{a.s.}$$

Remarks:

- The convergence theorem indicates the marginal distribution at a future time is close to the stationary distribution (in terms of replications of the chain).
- The ergodic theorem indicates the partial sample from a long chain is close to the stationary distribution.

Detailed Balance

- A distribution π is **detailed balanced** for a Markov chain with transition matrix P if
$$\pi(i)P_{ij} = \pi(j)P_{ji}, \quad \forall i, j.$$
- A detailed balanced distribution is a stationary distribution. (Not vice versa!)

Detailed Balance

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- A detailed balanced distribution is a stationary distribution. (Not vice versa!)
- Example: unique stationary distribution that is not detailed balanced.
Consider a Markov chain with state space $\{1, 2, 3\}$ and transition matrix
$$P = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$
The stationary distribution is $\pi = (1/3, 1/3, 1/3)$, but it is not detailed balanced.

Markov Chain Simulation

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- We treat the values of the markov chain as samples from the target distribution.
- The chain is generated by the following steps:
  - Start from an initial state X_0.
  - At each step t, generate X_{t+1} from the conditional distribution $P(X_{t+1}|X_t)$.
  - Repeat the above step for n steps.
  - The samples $\{X_0, X_1, \ldots, X_n\}$ are the samples from the target distribution.

The Metropolis Algorithm

Assume the target distribution is $\pi(x)$. The Metropolis algorithm generates a Markov chain with the following steps:

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- Start from an initial state X_0.
- At each step t, generate a candidate state Y from a **symmetric proposal** distribution $q(x, y)$.
- Compute the acceptance probability

$$\alpha(x, y) = \min\left\{1, \frac{\pi(y)}{\pi(x)}\right\}.$$

- Generate X_{t+1} by

$$X_{t+1} = \begin{cases} Y & \text{with probability } \alpha(x, y), \\ X_t & \text{with probability } 1 - \alpha(x, y). \end{cases}$$

- Repeat the above step for n steps.

The Metropolis Algorithm

Justification on the stationary distribution:

- The transition probability from x to y is

$$P(x, y) = \min\left\{1, \frac{\pi(y)}{\pi(x)}\right\}$$

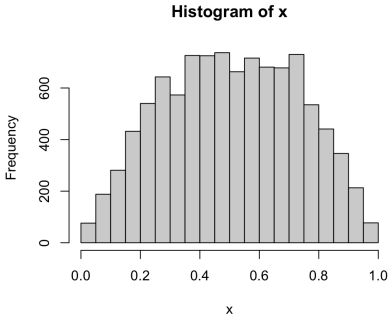
- The target distribution satisfies the detailed balance condition:

$$\pi(x)P(x, y) = \pi(y)P(y, x).$$

Implementation in R

Example: draw samples from $\mathrm{Beta}(2, 2)$ distribution.

```
n = 10000
x = rep(0, n+1)
x[1] = 0.5
for(i in 1:n){
    y = x[i] + rnorm(1) * 0.5
    a = dbeta(y, 2, 2) / dbeta(x[i],
        2, 2)
    if (runif(1) <= a) x[i+1] = y
    else x[i+1] = x[i]
}
```



Implementation in R

Update: Use random starting point.

```
n = 10000
x = rep(0, n+1)
x[1] = runif(1)
for(i in 1:n){
    y = x[i] + rnorm(1) * 0.5
    a = dbeta(y, 2, 2) / dbeta(x[i],
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}
```

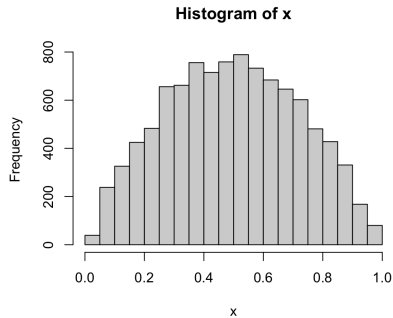

Implementation in R

Update: Add burnin period to get samples under convergence.

```
n = 10000
burnin = 1000
x = rep(0, n+1)
x0 = 0.5
for (i in 1:burnin){
    y = x0 + rnorm(1) * 0.5
    a = dbeta(y, 2, 2) / dbeta(x0,
        2, 2)
    if (runif(1) <= a) x0 = y
}
x[1] = x0
for(i in 1:n){
    y = x[i] + rnorm(1) * 0.5
    a = dbeta(y, 2, 2) / dbeta(x[i],
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}
```
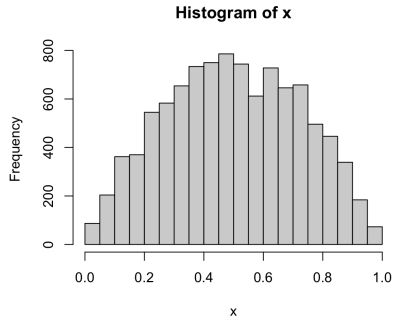



Implementation in R

Update: Encapsulate the code into a function.

```
metropolis <- function(target, n, burnin, proposal, initial){
    sample = rep(0, n)
    x = initial()
    for(i in 1:(n+burnin)){
        y = proposal(x)
        a = target(y) / target(x)
        if(runif(1) <= a) x = y
        if(i>burnin)
            sample[i-burnin] = x
    }
    return(sample)
}

target = function(x){dbeta(x, 2, 2)}
proposal = function(x){x + rnorm(1)*0.5}
initial = function(){runif(1)}
s = metropolis(target, n, burnin, proposal, initial)
```

Implementation in R

Update: Use log density for higher precision.

```
metropolis.log <- function(log.target, n, burnin, proposal, initial){
    sample = rep(0, n)
    x = initial()
    for(i in 1:(n+burnin)){
        y = proposal(x)
        du = log.target(y) - log.target(x)
        if(runif(1) <= exp(du)) x = y
        if(i>burnin) sample[i-burnin] = x
    }
    return(sample)
}

log.target = function(x){dbeta(x, 2, 2, log=T)}
proposal = function(x){x + rnorm(1)*0.5}
initial = function(){runif(1)}
s = metropolis.log(log.target, n, burnin, proposal, initial)
```

Implementation in R

Update: Allow parallel sampling with multiple chains

```
metropolis <- function(log.target, n, burnin, proposal, initial, n.chain)
    {
    sample = array(dim=c(n.chain, n))
    x = initial(n.chain)
    for(i in 1:(n+burnin)){
        y = proposal(x)
        du = log.target(y) - log.target(x)
        accept = runif(n.chain) <= exp(du)
        x[accept] = y[accept]
        if(i>burnin) sample[,i-burnin] = x
    }
    return(sample)
}

log.target = function(x){dbeta(x, 2, 2, log=T)}
proposal = function(x){x + rnorm(length(x))*0.5}
initial = function(n){runif(n)}
s = metropolis(log.target, n, burnin, proposal, initial, 4)
```

Perofrmance of Simulating Mutliple Chain

```
for(n.chain in 0:6){
    start = Sys.time()
    for(i in 1:100)
        s = metropolis(log.target, n, burnin, proposal, initial,
                       2**n.chain)
    end = Sys.time()
    print(c(2 ** n.chain, (end-start)/100))
}
```

- Resutls on my laptop, M1 Pro (8-core CPU):

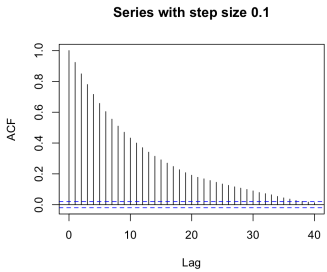
n.chain	1	2	4	8	16	32	64
time (ms)	53	58	65	79	107	173	298

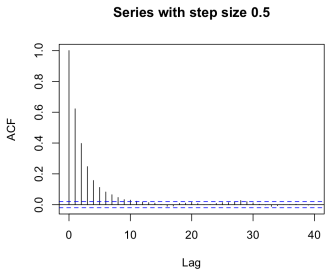
- Results on my desktop, 12900K (16-core CPU):

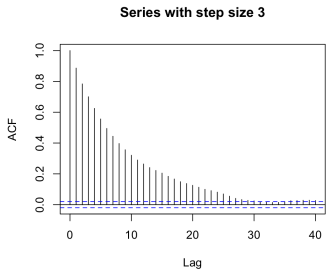
n.chain	1	2	4	8	16	32	64
time (ms)	34	40	44	52	69	106	176

Samples from the Metropolis Algorithm

Samples from the Metropolis algorithm are correlated.







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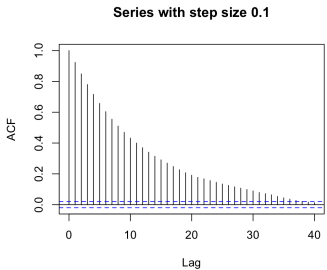

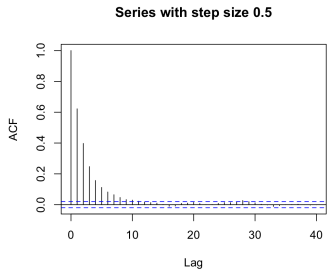

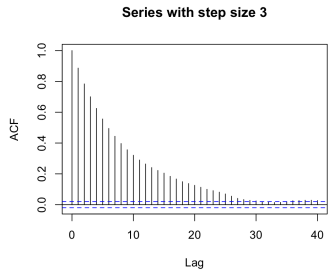

- A more local proposal distribution increases the autocorrelation.
- A more global proposal distribution resulting lower jumps increases the autocorrelation as well.
- One solution is to have asymmetric proposal distribution.

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- Start from an initial state X_0.
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- Compute the acceptance probability

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

- Generate X_{t+1} by

$$X_{t+1} = \begin{cases} Y & \text{with probability } \alpha(x, y), \\ X_t & \text{with probability } 1 - \alpha(x, y). \end{cases}$$

- Repeat the above step for n steps.

Implementation in R

```
metropolis.hastings <- function(log.target, n, burnin, proposal, initial,
     n.chain){
    sample = array(dim=c(n.chain, n))
    x = initial(n.chain)
    for(i in 1:(n+burnin)){
        prop = proposal(x)
        du = log.target(prop$y) - log.target(x)
        accept = runif(n.chain) <= exp(du+prop$dlog)
        x[accept] = prop$y[accept]
        if(i>burnin) sample[,i-burnin] = x
    }
    return(sample)
}
proposal = function(x){
    y = (0.5+x)/2 + rnorm(length(x))*0.5
    dlog = dnorm(x, (0.5+y)/2, 0.25, log=T) - dnorm(y, (0.5+x)/2, 0.25,
        log=T)
    return(list(y=y, dlog=dlog))
}
s = metropolis.hastings(log.target, n, burnin, proposal, initial, 1)
```

Comparison of Metropolis vs Metropolis-Hastings

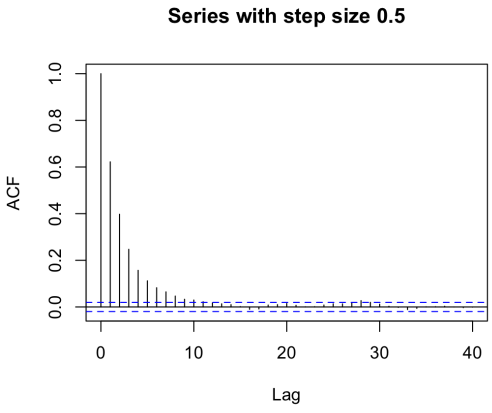

Figure: $q(x, y) = \mathcal{N}(x, 0.5^2)$

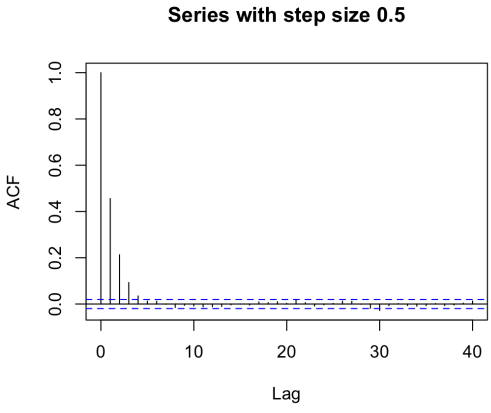

Figure: $q(x, y) = \mathcal{N}\left(\frac{x+0.5}{2}, 0.5^2\right)$