

CS492: Probabilistic Programming

Markov Chain

Monte Carlo

Hongseok Yang

KAIST

CS492: Probabilistic Programming

Markov Chain

Monte Carlo



Hongseok Yang
KAIST

Really about: Metropolis-Hastings algorithm

```
(doquery :1mh induce-fn [ints2 outs2])
```

(doquery :**lmh** induce-fn [ints2 outs2])



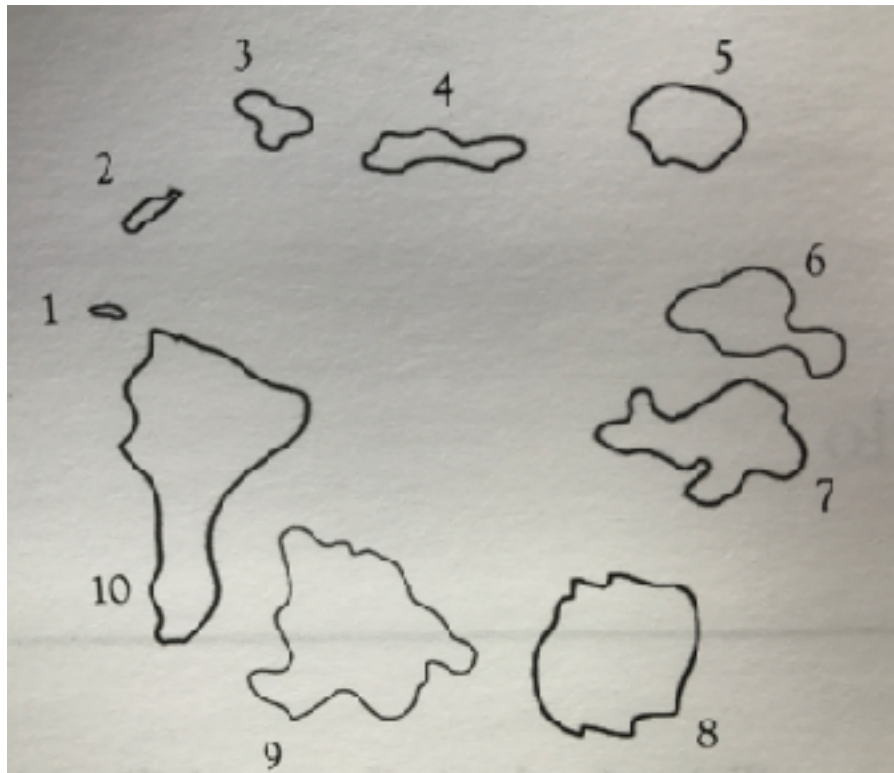
Lightweight Metropolis Hastings algorithm* (LMH).

* Wingate, Stuhlmuller and Goodman's paper at AISTATS 2011

Learning outcome

- Can explain Metropolis-Hastings algorithm.
- Can say when this algo. is correct.
- Can develop an instance of the algorithm.

Good king Markov puzzle*

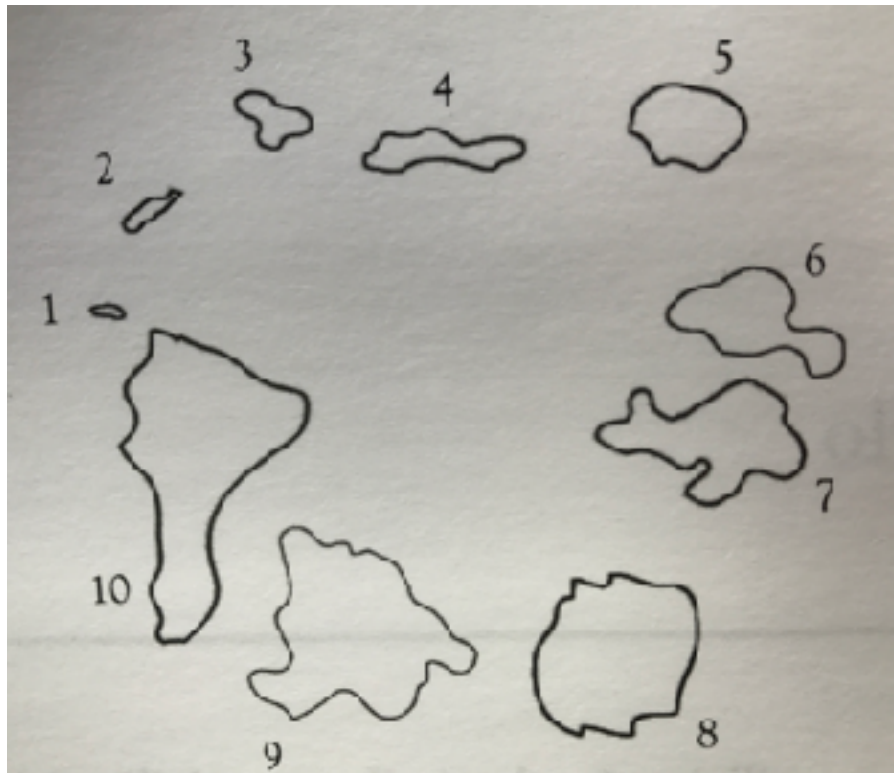


Markov rules 10 islands.

$100i$ people live in island i .

* Borrowed from McElreath's book "Statistical Rethinking"

Good king Markov puzzle*



Markov rules 10 islands.

$100i$ people live in island i .

King loves his people and wants to visit each island in proportion to its population size.

[Q] Find an algorithm. No scheduling nor bookkeeping. Can move adjacent islands only.

* Borrowed from McElreath's book "Statistical Rethinking"

Good king Markov puzzle*

Bad!!



Markov rules 10 islands.

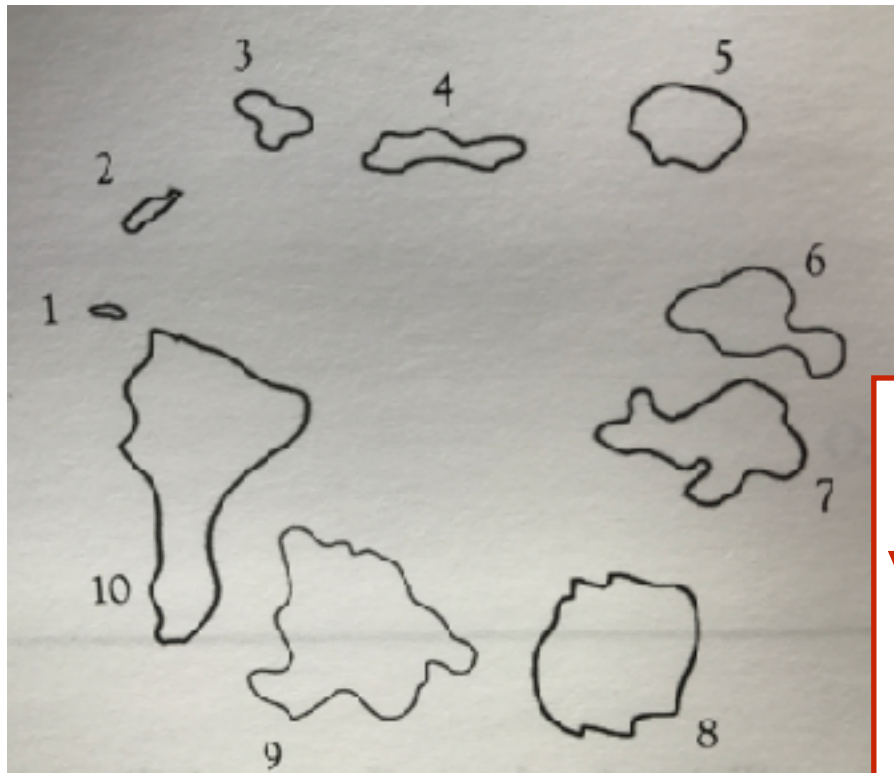
$100i$ people live in island i .

King loves his people and wants to visit each island in proportion to its population size.

[Q] Find an algorithm. **No scheduling nor bookkeeping.** Can move adjacent islands only.

* Borrowed from McElreath's book "Statistical Rethinking"

Good king Markov puzzle*



Markov rules 10 islands.

$100i$ people live in island i .

$i \sim \text{discrete}(1, 2, \dots, 10)$.
Visit i .
Repeat.

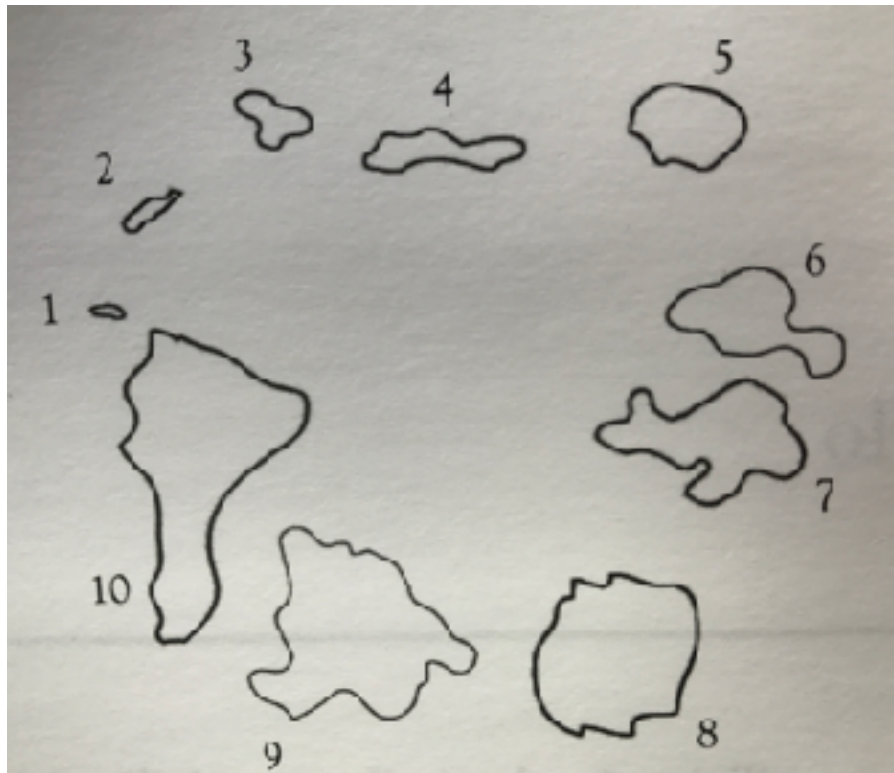
Bad!!

King loves his people and wants to visit each island in proportion to its population size.

[Q] Find an algorithm. No scheduling nor bookkeeping. **Can move adjacent islands only.**

* Borrowed from McElreath's book "Statistical Rethinking"

Good king Markov puzzle*



Markov rules 10 islands.

$100i$ people live in island i .

King loves his people and wants to visit each island in proportion to its population size.

[Q] Find an algorithm. No scheduling nor bookkeeping. Can move adjacent islands only.

* Borrowed from McElreath's book "Statistical Rethinking"

Solution

k_n — island that the king visits at step n .

Repeat the following steps:

1. Flip a coin with prob. 0.5. If head, pick next k' clockwise. If tail, use k' counterclockwise.
2. $\alpha := \min(1, k'/k_n)$.
3. Flip a coin with prob. α . If head, $k_{n+1} := k'$. Otherwise, $k_{n+1} := k_n$.

Solution

k_n — island that the king visits at step n .

Repeat the following steps:

1. Flip a coin with prob. 0.5. If head, pick next k' clockwise. If tail, use k' counterclockwise.
2. $\alpha := \min(1, k'/k_n)$.
3. Flip a coin with prob. α . If head, $k_{n+1} := k'$. Otherwise, $k_{n+1} := k_n$.

[Q] Why correct? What does correctness even mean?

Sequence by the algo.: $k_1, k_2, \dots, k_n, \dots$

Sequence by the algo.: $k_1, k_2, \dots, k_n, \dots$

[Strong convergence] For any $f : \{1, \dots, 10\} \rightarrow \mathbb{R}$,
 $(\sum_{j \leq n} f(k_j))/n \rightarrow \mathbb{E}_{p(i)}[f(i)]$ as $n \rightarrow \infty$ with prob. 1,
where $p(i) = i/55$, target prob. for visiting island i .

Intuitively, frequency represents probability.

Sequence by the algo.: $k_1, k_2, \dots, k_n, \dots$

[Strong convergence] For any $f : \{1, \dots, 10\} \rightarrow \mathbb{R}$,
 $(\sum_{j \leq n} f(k_j))/n \rightarrow \mathbb{E}_{p(i)}[f(i)]$ as $n \rightarrow \infty$ with prob. 1,
where $p(i) = i/55$, target prob. for visiting island i .

Intuitively, frequency represents probability.

Holds because 1) the random move of the algo.
has p as **invariant**; 2) the algo. can **move**
between any two islands in finitely many steps.

Sequence by the algo.: $k_1, k_2, \dots, k_n, \dots$

[Strong convergence] For any $f : \{1, \dots, 10\} \rightarrow \mathbb{R}$,
 $(\sum_{j \leq n} f(k_j))/n \rightarrow \mathbb{E}_{p(i)}[f(i)]$ as $n \rightarrow \infty$ with prob. 1,
where $p(i) = i/55$, target prob. for visiting island i .

Intuitively, frequency represents probability.

Holds because 1) the random move of the algo.
has p as invariant; 2) the algo. can move
between any two islands in finitely many steps.

[Q] Prove 1) and 2).

Metropolis algorithm

Goal: Generate samples from target $r(x)/Z$, where $Z = \int r(x)dx$, the normalising constant.

Parameter: Conditional distribution $q(x'|x)$.

- Should be symmetric $q(x'|x) = q(x|x')$.
- Represents a random move.
- Called proposal kernel.

Metropolis algorithm

Goal: Generate samples from target $r(x)/Z$, where $Z = \int r(x)dx$, the normalising constant.

Parameter: Conditional distribution $q(x'|x)$.

- Should be symmetric $q(x'|x) = q(x|x')$.
- Represents a random move.
- Called proposal kernel.

[Q] What are $r(-)$ and $q(-|-)$ in King Markov?

Metropolis algorithm

Target $r(x)/Z$. Symmetric proposal $q(x'|x)$.

1. initialise x_1 randomly; $n:=1$
2. repeat:
 - a) $x' \sim q(x'|x_n)$; $\alpha := \min(1, r(x')/r(x_n))$
 - b) $u \sim \text{uniform}(0,1)$
 - c) $x_{n+1} := (\text{if } (u \leq \alpha) \text{ then } x' \text{ else } x_n)$; $n:=n+1$

Metropolis

Noisy greedy exploration.

Target $r(x)/Z$. Symmetric proposal $q(x'|x)$.

1. initialise x_1 randomly; $n:=1$
2. repeat:
 - a) $x' \sim q(x'|x_n)$; $\alpha := \min(1, r(x')/r(x_n))$
 ≥ 1 for better x'
 < 1 for worse x'
 - b) $u \sim \text{uniform}(0,1)$
 - c) $x_{n+1} := (\text{if } (u \leq \alpha) \text{ then } x' \text{ else } x_n)$; $n:=n+1$

Metropolis

Noisy greedy exploration.
No need to know Z .

Target $r(x)/Z$. Symmetric proposal $q(x'|x)$.

1. initialise x_1 randomly; $n:=1$
2. repeat:
 - a) $x' \sim q(x'|x_n)$; $\alpha := \min(1, r(x')/r(x_n))$
 - b) $u \sim \text{uniform}(0,1)$
 - c) $x_{n+1} := (\text{if } (u \leq \alpha) \text{ then } x' \text{ else } x_n)$; $n:=n+1$

Metropolis

Noisy greedy exploration.
No need to know Z .

Target $r(x)/Z$. Symmetric proposal $q(x'|x)$.

1. initialise x_1 randomly; $n:=1$
2. repeat:
 - a) $x' \sim q(x'|x_n)$; $\alpha := \min(1, r(x')/r(x_n))$
 - b) $u \sim \text{uniform}(0,1)$
 - c) $x_{n+1} := (\text{if } (u \leq \alpha) \text{ then } x' \text{ else } x_n)$; $n:=n+1$

[Q1] How is it related to our sol. for King Markov?

Metropolis

Noisy greedy exploration.
No need to know Z .

Target $r(x)/Z$. Symmetric proposal $q(x'|x)$.

1. initialise x_1 randomly; $n:=1$
2. repeat:
 - a) $x' \sim q(x'|x_n)$; $\alpha := \min(1, r(x')/r(x_n))$
 - b) $u \sim \text{uniform}(0,1)$
 - c) $x_{n+1} := (\text{if } (u \leq \alpha) \text{ then } x' \text{ else } x_n)$; $n:=n+1$

[Q2] Use it & do posterior inference. Assume $x \in \mathbb{R}^m$.

$$r(x) = p(y|x)p(x)$$

$$q(x'|x) = \text{normal}(x, \varepsilon \times \text{ID})$$

Noisy greedy exploration.

No need to know Z .

Target $r(x)/Z$. Symmetric proposal $q(x'|x)$.

1. initialise x_1 randomly; $n:=1$

2. repeat:

a) $x' \sim q(x'|x_n)$; $\alpha := \min(1, r(x')/r(x_n))$

b) $u \sim \text{uniform}(0,1)$

c) $x_{n+1} := (\text{if } (u \leq \alpha) \text{ then } x' \text{ else } x_n)$; $n:=n+1$

[Q2] Use it & do posterior inference. Assume $x \in \mathbb{R}^m$.

Metropolis

Noisy greedy exploration.
No need to know Z .

Target $r(x)/Z$. Symmetric proposal $q(x'|x)$.

1. initialise x_1 randomly; $n:=1$

2. repeat:

a) $x' \sim q(x'|x_n)$; $\alpha := \min(1, r(x')/r(x_n))$

b) $u \sim \text{uniform}(0,1)$

c) $x_{n+1} := (\text{if } (u \leq \alpha) \text{ then } x' \text{ else } x_n)$; $n:=n+1$

[Q3] Does each step preserve $r(x)/Z$ as invariant?

Metropolis

Noisy greedy exploration.
No need to know Z .

Target $r(x)/Z$. Symmetric proposal $q(x'|x)$.

1. initialise x_1 randomly; $n:=1$
2. repeat:
 - a) $x' \sim q(x'|x_n)$; $\alpha := \min(1, r(x')/r(x_n))$
 - b) $u \sim \text{uniform}(0,1)$
 - c) $x_{n+1} := (\text{if } (u \leq \alpha) \text{ then } x' \text{ else } x_n)$; $n:=n+1$

[Q4] Instantiate this algo. for Anglican programs.

Hastings Metropolis algorithm

Target $r(x)/Z$. ~~Symmetric~~ proposal $q(x'|x)$.

1. initialise x_1 randomly; $n:=1$

2. repeat:

a) $x' \sim q(x'|x_n)$; $\alpha := \min(1, \frac{r(x') \times q(x_n|x')}{r(x_n) \times q(x'|x_n)})$

b) $u \sim \text{uniform}(0,1)$

c) $x_{n+1} := (\text{if } (u \leq \alpha) \text{ then } x' \text{ else } x_n); \quad n:=n+1$

Hastings Metropolis algorithm

Target $r(x)/Z$. ~~Symmetric~~ proposal $q(x'|x)$.

1. initialise x_1 randomly; $n:=1$

2. repeat:

a) $x' \sim q(x'|x_n)$; $\alpha := \min(1, \frac{r(x') \times q(x_n|x')}{r(x_n) \times q(x'|x_n)})$

b) $u \sim \text{uniform}(0,1)$

c) $x_{n+1} := (\text{if } (u \leq \alpha) \text{ then } x' \text{ else } x_n)$; $n:=n+1$

[Q1] Develop q for the King Markov puzzle.

Hastings Metropolis algorithm

Target $r(x)/Z$. ~~Symmetric~~ proposal $q(x'|x)$.

1. initialise x_1 randomly; $n:=1$

2. repeat:

a) $x' \sim q(x'|x_n)$; $\alpha := \min(1, \frac{r(x') \times q(x_n|x')}{r(x_n) \times q(x'|x_n)})$

b) $u \sim \text{uniform}(0,1)$

c) $x_{n+1} := (\text{if } (u \leq \alpha) \text{ then } x' \text{ else } x_n); \quad n:=n+1$

[Q2] Noisy greedy exploration. Find a (relative) obj.

Hastings Metropolis algorithm

Target $r(x)/Z$. ~~Symmetric~~ proposal $q(x'|x)$.

1. initialise x_1 randomly; $n:=1$

2. repeat:

a) $x' \sim q(x'|x_n)$; $\alpha := \min(1, \frac{r(x') \times q(x_n|x')}{r(x_n) \times q(x'|x_n)})$

b) $u \sim \text{uniform}(0,1)$

c) $x_{n+1} := (\text{if } (u \leq \alpha) \text{ then } x' \text{ else } x_n); \quad n:=n+1$

[Q2] Noisy greedy exploration. Find a (relative) obj.

Hastings Metropolis algorithm

Target $r(x)/Z$. ~~Symmetric~~ proposal $q(x'|x)$.

1. initialise x_1 randomly; $n:=1$

2. repeat:

a) $x' \sim q(x'|x_n)$; $\alpha := \min(1, \frac{r(x') \times q(x_n|x')}{r(x_n) \times q(x'|x_n)})$

b) $u \sim \text{uniform}(0,1)$

c) $x_{n+1} := (\text{if } (u \leq \alpha) \text{ then } x' \text{ else } x_n); \quad n:=n+1$

[Q3] Does each step preserve $r(x)/Z$ as invariant?

Recap of the MH algo.

- Generate samples from unnormalised $r(x)$.
No need to know $Z = \int r(x) dx$.
- Noisy greedy exploration using $q(x'|x)$.

Guarantees informally

[Thm I] Each step of MH has r/Z as inv. dist.

Guarantees informally

MH samples: $x_1, x_2, x_3, \dots, x_n, \dots$

[Thm2] For all $f: X \rightarrow \mathbb{R}$ with $\mathbb{E}_{r(x)/Z}[f(x)]$ defined,

$\sum_{i \leq n} f(x_i)/n \rightarrow \mathbb{E}_{r(x)/Z}[f(x)]$ as $n \rightarrow \infty$ with prob. 1,

if the MH with q is r/Z -irreducible.

Guarantees informally

The estimate converges to the right value.

MH samples: $x_1, x_2, x_3, \dots, x_n, \dots$

[Thm2] For all $f: X \rightarrow \mathbb{R}$ with $\mathbb{E}_{r(x)/Z}[f(x)]$ defined,

$\sum_{i \leq n} f(x_i)/n \rightarrow \mathbb{E}_{r(x)/Z}[f(x)]$ as $n \rightarrow \infty$ with prob. 1,

if the MH with q is r/Z -irreducible.

Guarantees informally

The estimate converges to the right value.

MH samples: $x_1, x_2, x_3, \dots, x_n, \dots$

[Thm2] For all $f: X \rightarrow \mathbb{R}$ with $\mathbb{E}_{r(x)/Z}[f(x)]$ defined,

$\sum_{i \leq n} f(x_i)/n \rightarrow \mathbb{E}_{r(x)/Z}[f(x)]$ as $n \rightarrow \infty$ with prob. 1,

if the MH with q is r/Z -irreducible.

MH moves well. For any r/Z -possible x, x' , the MH can go from x to x' with non-zero prob.

Guarantees informally

The estimate converges to the right value.

MH samples: $x_1, x_2, x_3, \dots, x_n, \dots$

[Thm2] For all $f: X \rightarrow \mathbb{R}$ with $\mathbb{E}_{r(x)/Z}[f(x)]$ defined,

$\sum_{i \leq n} f(x_i)/n \rightarrow \mathbb{E}_{r(x)/Z}[f(x)]$ as $n \rightarrow \infty$ with prob. 1,

if the MH with q is r/Z -irreducible.

MH moves well. For any r/Z -possible x, x' , the MH can go from x to x' with non-zero prob.

Guarantees informally

MH samples: $x_1, x_2, x_3, \dots, x_n, \dots$

[Thm2] For all $f: X \rightarrow \mathbb{R}$ with $\mathbb{E}_{r(x)/Z}[f(x)]$ defined,

$\sum_{i \leq n} f(x_i)/n \rightarrow \mathbb{E}_{r(x)/Z}[f(x)]$ as $n \rightarrow \infty$ with prob. 1,

if the MH with q is r/Z -irreducible.

Consequence of a general result in ergodic theory.
Thm1 plays a crucial role in the proof.

Reference

I looked at Chapters 5 and 6 of Robert & Casella's "Monte Carlo Statistical Methods".

Not recommended for general reading.

But details and pointers can be found there.