CS492: Probabilistic Programming

Markov Chain Monte Carlo

Hongseok Yang
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Really about: Metropolis-Hastings algorithm

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

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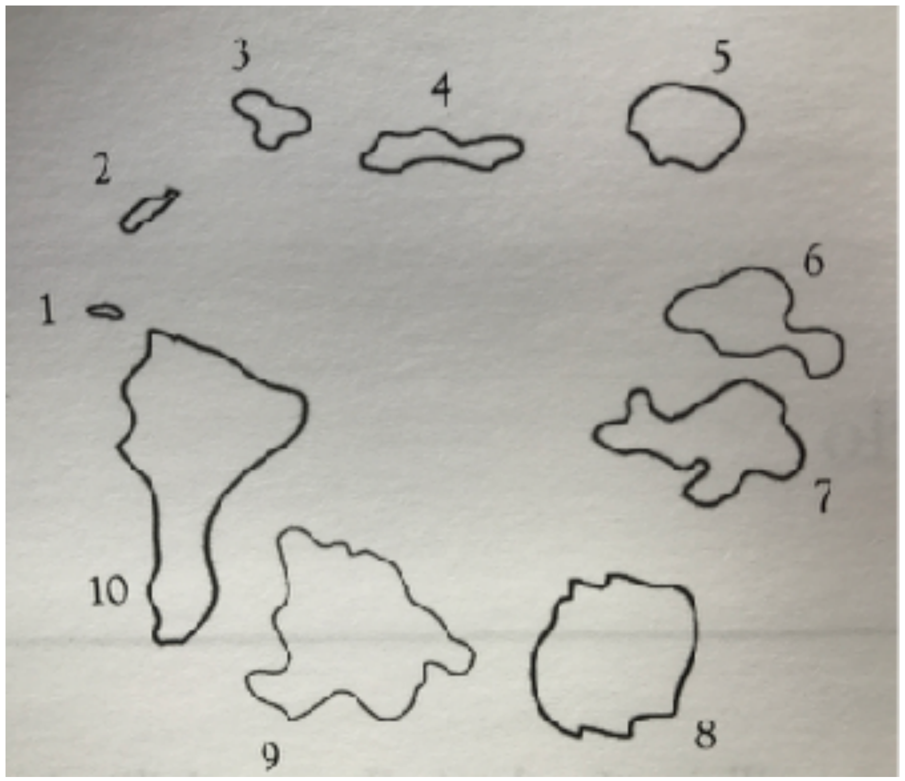
Lightweight Metropolis Hastings algorithm* (LMH).

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

Learning outcome

- Can explain Metropolis-Hastings algorithm.
- Can say when and why 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"

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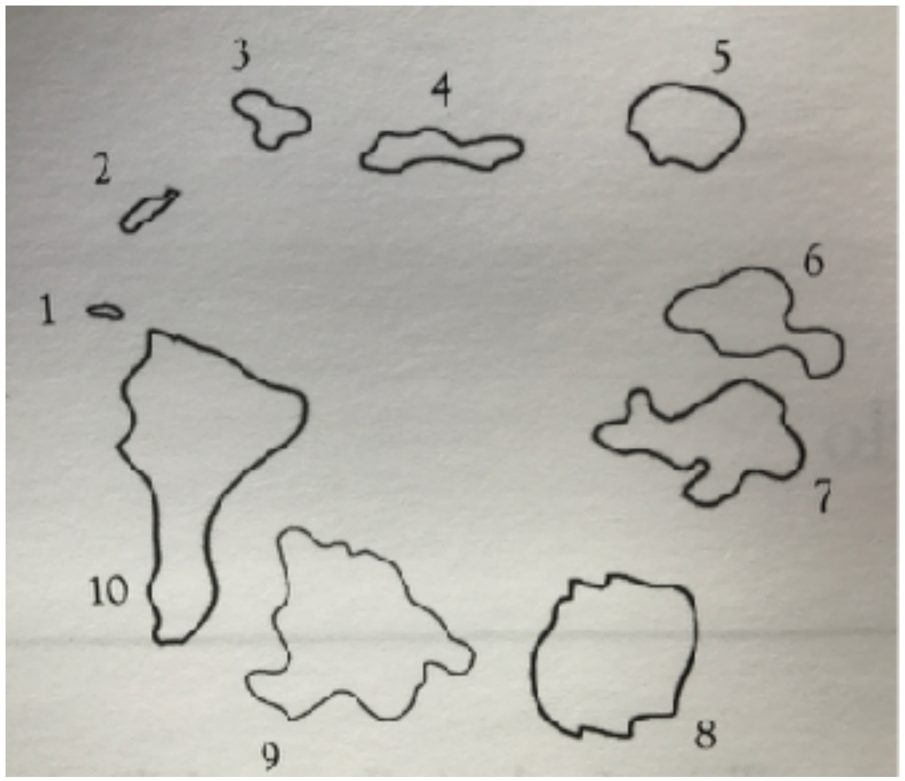

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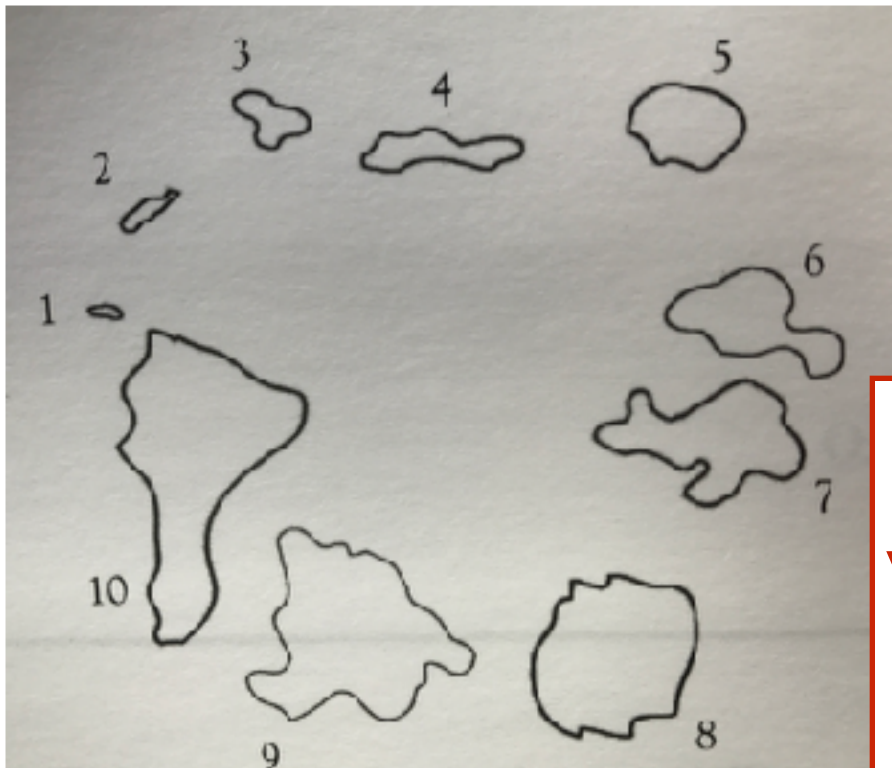

Markov rules 10 islands.

100i people live in island i.

i ~ discrete(1,2,...,10).
Visit i.
Repeat.

Bad!!

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

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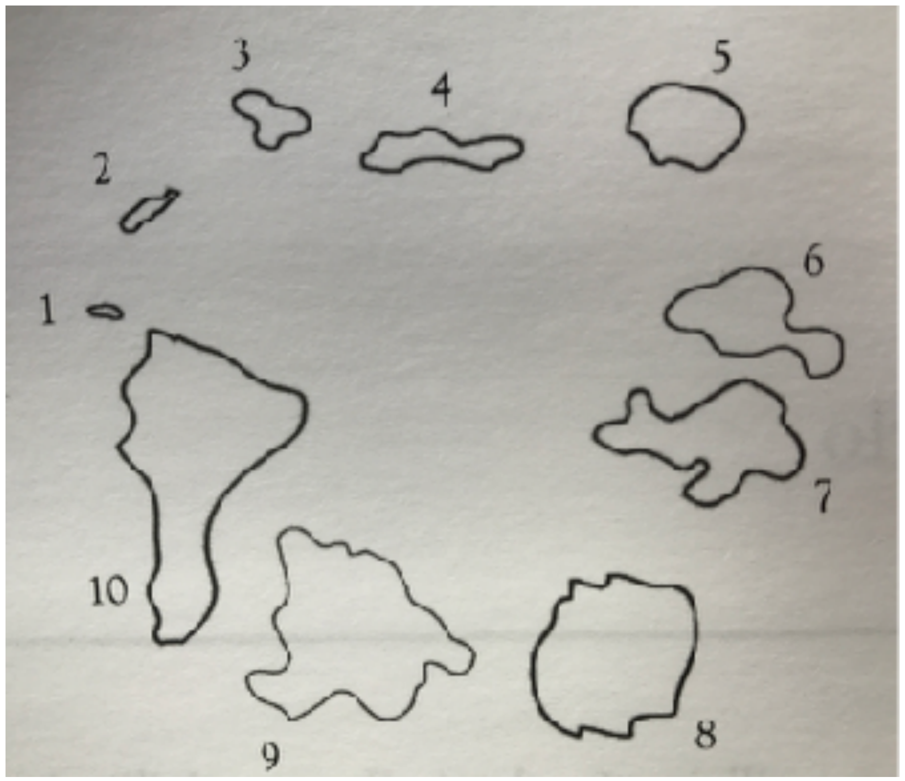

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Solution

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, $k_{n+1} := k_n$.

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

Sequence by the algo.: k_1, k_2, …, k_n, …

Corr. informally: Frequency represents probability.

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

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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 (>0) steps.

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

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[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.

E.g. $r(i)=i$, $Z=55$, $q(j|i)=0.5\times[(j-i) \bmod 10 \in \{1,0,-1\}]$

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

Metropolis

Noisy greedy exploration.

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

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Noisy greedy exploration.
No need to know Z.

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May use flip(α) instead, as in our sol. for King Markov

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[Q1] Does each step preserve $r(x)/Z$ as invariant?

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[Q2] Posterior inference. Latent $x \in \mathbb{R}^2$. Observed $y \in \mathbb{R}$

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[Q2] Posterior inference. Latent $x \in \mathbb{R}^2$. Observed $y \in \mathbb{R}$

$r(x) = p(y|x)p(x),$
$q(x'|x) = \text{normal}(x'_1|x_1,\varepsilon_1)$
$\times\ \text{normal}(x'_2|x_2,\varepsilon_2)$

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[Q3] How to instantiate this algo. for Anglican prog.?

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[Q3] How to instantiate this algo. for Anglican prog.?

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(defquery q []
  (let [x1  (sample (normal 0 1))
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[Q] Prior p(x) and likelihood p(y|x). What are the types of x and y?

(1) $x \in \mathbb{R}$, $y \in \mathbb{R}^2$

(2) $x \in \mathbb{R}^2$, $y \in \mathbb{R}^2$

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Prob. distr. on result

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Execute all sample exprs.
Prob. distr. on all samples.

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        b   (sample (normal (* x1 x1) 4))
        x2  (if (> x1 0) 1 b)]
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Prob. distr. on execution traces that record only sampled values.

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(defquery q []                      -0.9
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- All correct.
- (3) used for the design of MCMC for Anglican.

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$\boxed{-1.8}$ $\boxed{8.2}$

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0.9

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```

But q by re-execution is not symm.

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Metropolis Hastings algorithm

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

1. initialise x_1 randomly; $n:=1$
2. repeat:
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    b) $u \sim \text{uniform}(0,1)$
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[Q1] q by re-execution for Anglican. What is $q(x'|x)$?

Hastings
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   a) $x' \sim q(x'|x_n)$; $\alpha := \min\left(1, \cancel{r(x')/r(x_n)}\ \frac{r(x') \times q(x_n|x')}{r(x_n) \times q(x'|x_n)}\right)$
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   c) $x_{n+1} :=$ (if $(u \leq \alpha)$ then x' else x_n); $n{:=}n+1$

[Q1] q by re-execution for Anglican. What is $q(x'|x)$?

[A1] $q(x'|x) = p(x')$.

Metropolis Hastings algorithm

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

1. initialise x_1 randomly; $n{:=}1$
2. repeat:
   a) $x' \sim q(x'|x_n)$; $\alpha := \min(1, \cancel{r(x')/r(x_n)}\ \dfrac{r(x')\times q(x_n|x')}{r(x_n)\times q(x'|x_n)})$
   b) $u \sim \text{uniform}(0,1)$
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[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) $x' \sim q(x'|x_n)$; $\alpha := \min\left(1, \overbrace{\cancel{r(x')/r(x_n)}}^{\dfrac{r(x')\times q(x_n|x')}{r(x_n)\times q(x'|x_n)}}\right)$

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

$\overbrace{\text{Metropolis algorithm}}^{\text{Hastings}}$

Target r(x)/Z. ~~Symmetric~~ pro

When independent proposal is used.

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

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

Metropolis Hastings algorithm

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

1. initialise x_1 randomly; $n:=1$
2. repeat:
   a) $x' \sim q(x'|x_n)$; $\alpha := \min\left(1, \overbrace{\cancel{r(x')/r(x_n)}}^{\frac{r(x')\times q(x_n|x')}{r(x_n)\times q(x'|x_n)}}\right)$

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

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

[Q3] Does each step have $r(x)/Z$ 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

[Thm1] Each step of MH has r/Z as inv. dist.

Guarantees informally

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

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

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

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

Guarantees informally

The estimate converges to the right value.

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

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

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The estimate converges to the right value.

MH samples: x_1, x_2, x_3, …, x_n, …

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MH moves well. For any x,x' with r(x')>0, the MH can go from x to x' with non-zero prob.

Guarantees informally

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MH samples: x_1, x_2, x_3, …, x_n, …

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

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

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.