

# Markov Chain Monte Carlo

Felipe José Bravo Márquez

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# Markov Chain Monte Carlo

- This class introduces estimation of posterior probability distributions using a stochastic process known as **Markov chain Monte Carlo** (MCMC).
- Here we'll produce samples from the joint posterior without maximizing anything.
- We will be able to sample directly from the posterior without assuming a Gaussian, or any other, shape.
- The cost of this power is that it may take much longer for our estimation to complete.
- But the benefit is escaping multivariate normality assumption of the Laplace approximation.
- More advanced models such as the generalized linear and multilevel models tend produce non-Gaussian posterior distributions.
- In most cases they cannot be estimated at all with the techniques of earlier classes.
- This class is based on Chapter 9 of [McElreath, 2020] and Chapter 7 of [Kruschke, 2014].

# Markov Chain Monte Carlo

- The essence of MCMC is to produce samples from the posterior  $f(\theta|d)$  by only accessing a function that is proportional to it.
- This proportional function is the product of the likelihood and the prior  $f(d|\theta) * f(\theta)$ , which is always available in a Bayesian model.
- So, merely by evaluating  $f(d|\theta) * f(\theta)$ , without normalizing it by  $f(d)$ , MCMC allows us to generate random representative values from the posterior distribution.
- This property is wonderful because the method obviates direct computation of the evidence  $f(d)$ , which, as you'll recall, is one of the most difficult aspects of Bayesian inference.
- It has only been with the development of MCMC algorithms and software that Bayesian inference is applicable to complex data analysis.
- And it has only been with the production of fast and cheap computer hardware that Bayesian inference is accessible to a wide audience.
- The question then becomes this: How does MCMC work? For an answer, let's ask a politician.

# A politician stumbles upon the Metropolis algorithm

- Suppose an elected politician lives on a long chain of islands.
- He is constantly traveling from island to island, wanting to stay in the public eye.
- At the end of a day he has to decide whether to:
  - 1 stay on the current island
  - 2 move to the adjacent island to the west
  - 3 move to the adjacent island to east
- His goal is to visit all the islands **proportionally** to their **relative population**.
- But, he doesn't know the total population of all the islands.
- He only knows the population of the current island where he is located.
- He can also ask about the population of an adjacent island to which he plans to move.

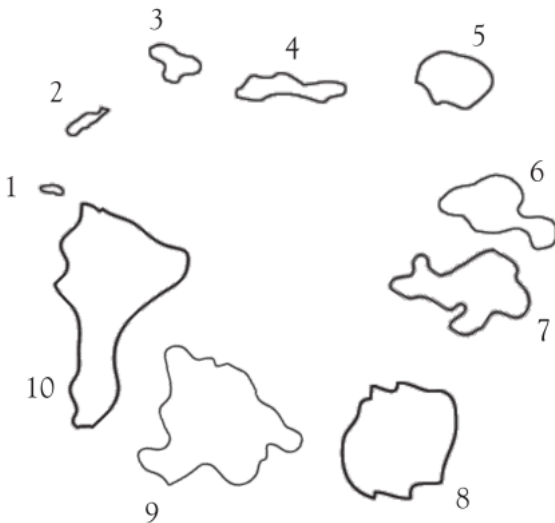
# The Metropolis algorithm

- The politician has a simple heuristic for travelling accross the islands called the **Metropolis** algorithm.
- First, he flips a (fair) coin to decide whether to propose the adjacent island to the left or the adjacent island to the right.
- If the proposed island has a larger population than the current island ( $P_{proposed} > P_{current}$ ), then he goes to the proposed island.
- If the proposed island has a smaller population than the current island ( $P_{proposed} < P_{current}$ ), then he goes to the proposed island with probability  $p_{move} = P_{proposed} / P_{current}$ .
- In the long run, the probability that the politician is on any one of the islands exactly matches the relative population of the island!

# The Metropolis algorithm

- Let's analyze the Metropolis algorithm in more detail.
- Suppose there are 10 islands in total.
- Each island is neighbored by two others, and the entire archipelago forms a ring.
- The islands are of different sizes, and so had different sized populations living on them.
- The second island is twice as populous as the first, the third three times as populous as the first.
- And so on, up to the largest island, which is 10 times as populous as the smallest.

# The Metropolis algorithm



# The Metropolis algorithm

- We are going to show an implementation of this algorithm in R.
- But before that, we will combine combine the two possibilities: the proposed island having a 1) higher or 2) lower population than the current island, into a single expression:

$$p_{\text{move}} = \min(1, P_{\text{proposed}}/P_{\text{current}}). \quad (1)$$

- So, if  $P_{\text{proposed}} > P_{\text{current}}$ ,  $P_{\text{proposed}}/P_{\text{current}} > 1$  and  $p_{\text{move}} = 1$ .
- For example,  $\text{current} = 4$  and  $\text{proposed} = 5$ ,  $5/4 > 1$  so we move to the proposed island.
- On the other hand, if  $P_{\text{proposed}} < P_{\text{current}}$ ,  $P_{\text{proposed}}/P_{\text{current}} < 1$ , and  $p_{\text{move}} = P_{\text{proposed}}/P_{\text{current}}$ .
- For example,  $\text{current} = 4$  and  $\text{proposed} = 3$ ,  $3/4 < 1$  so we move to the proposed island with probability  $3/4$ .

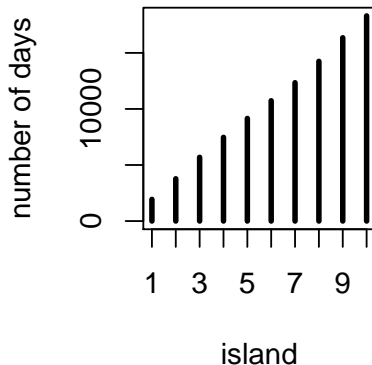


# The Metropolis algorithm

```
num_days <- 1e5
positions <- rep(0,num_days)
current <- 10
for ( i in 1:num_days ) {
  # record current position
  positions[i] <- current
  # flip coin to generate proposal
  proposal <- current + sample( c(-1,1) , size=1 )
  # now make sure he loops around the archipelago
  if ( proposal < 1 ) proposal <- 10
  if ( proposal > 10 ) proposal <- 1
  # move?
  prob_move <- min(proposal/current,1)
  decision <- rbinom(1,1,prob_move)
  current <- ifelse( decision == 1 , proposal , current )
}

library(rethinking)
simplehist(positions,xlab="island",ylab="number of days")
```

# The Metropolis algorithm



The time spent on each island is proportional to its population size.

# The Metropolis algorithm

- The first three lines of the method just define the number of days to simulate, an empty history vector, and a starting island position (the biggest island, number 10).
- Then the for loop steps through the days.
- Each day, it records the politician's current position.
- Then it simulates a coin flip to nominate a proposal island.
- The only trick here lies in making sure that a proposal of "11" loops around to island 1 and a proposal of "0" loops around to island 10.
- Finally, a random binary number is generated with a binomial distribution with probability of success (or moving) =  $\min(1, P_{proposed} / P_{current})$
- If this random number is 1 we move, otherwise we stay.

# The Metropolis algorithm

- In real applications, the goal is of course not to help a politician, but instead to draw samples from an unknown and usually complex posterior probability distribution.
- The “islands” in our objective are parameter values  $\theta$ , and they need not be discrete, but can instead take on a continuous range of values as usual.
- The “population sizes” in our objective are the posterior probabilities (or densities) at each parameter value:  $f(\theta|d)$
- The “days” in our objective are samples taken from the posterior distribution.
- The Metropolis algorithm will eventually give us a collection of samples from the posterior.
- We can then use these samples just like all the samples we have already used in this course.

# Why it works

- Now, let's try to understand the mathematics behind why the algorithm works.
- Consider two adjacent positions and the probabilities of moving from one to the other.
- We'll see that the relative transition probabilities, between adjacent positions, exactly match the relative values of the target distribution.
- Extrapolate that result across all the positions, and you can see that, in the long run, each position will be visited proportionally to its target value.
- Suppose we are at position  $\theta$ .
- The probability of moving to  $\theta + 1$ , denoted  $P(\theta \rightarrow \theta + 1)$ , is the probability of proposing that move times the probability of accepting it if proposed, which is:

$$P(\theta \rightarrow \theta + 1) = 0.5 \times \min(P(\theta + 1)/P(\theta), 1)$$

# Conclusions

- Blabla

# References I



Kruschke, J. (2014).

Doing bayesian data analysis: A tutorial with r, jags, and stan.



McElreath, R. (2020).

*Statistical rethinking: A Bayesian course with examples in R and Stan.*  
CRC press.