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 to 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 proportial to it.
- This proportial 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 an 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 left
  3. move to the adjacent island to right
- 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.

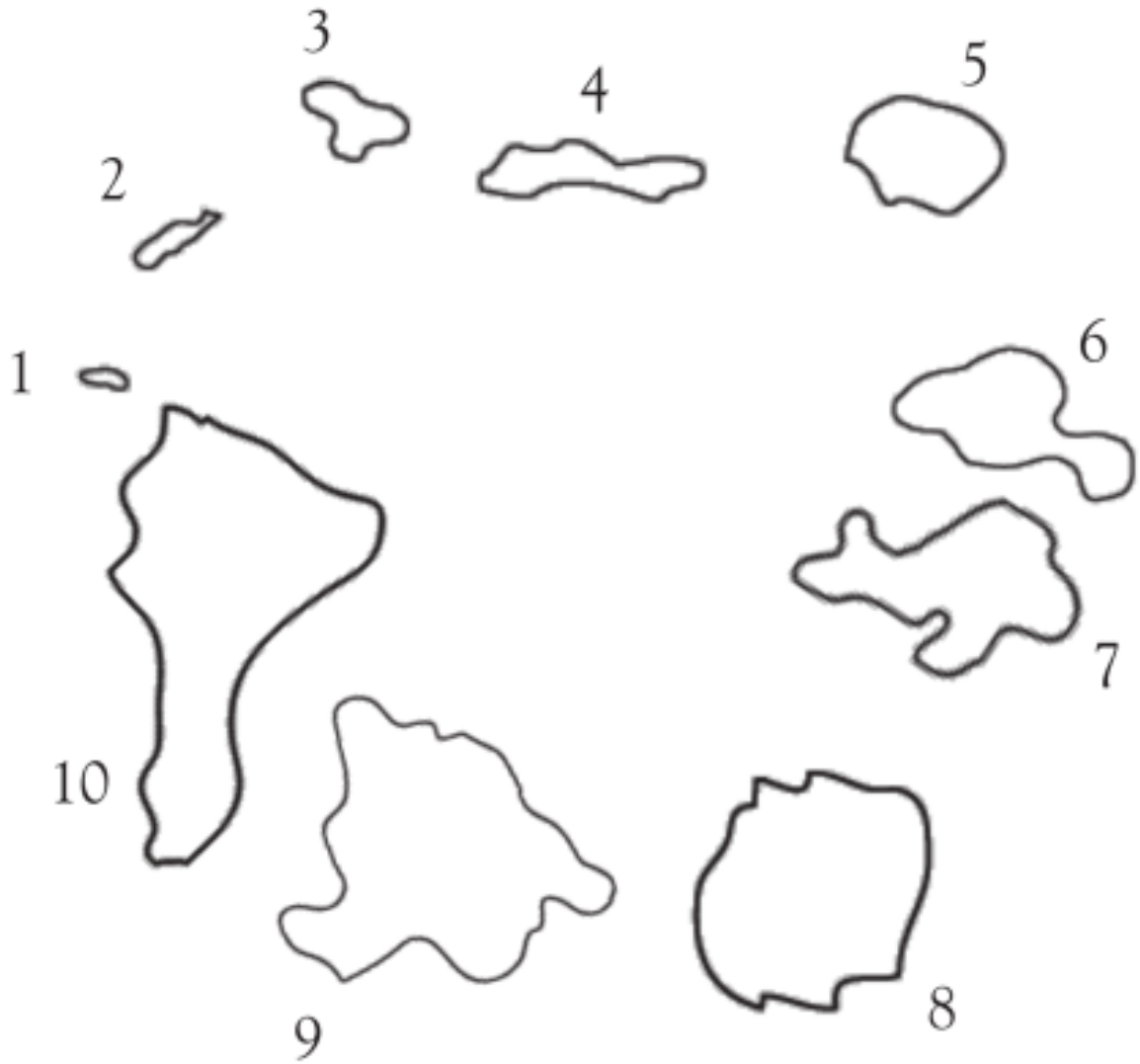
The Metropolis algorithm

- The politician has a simple heuristic for travelling accross the islands called the **Metropolis** algorithm [Metropolis et al., 1953].
- 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 for the probability of moving into a single expression: the proposed island having a 1) higher or 2) lower population than the current island.

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

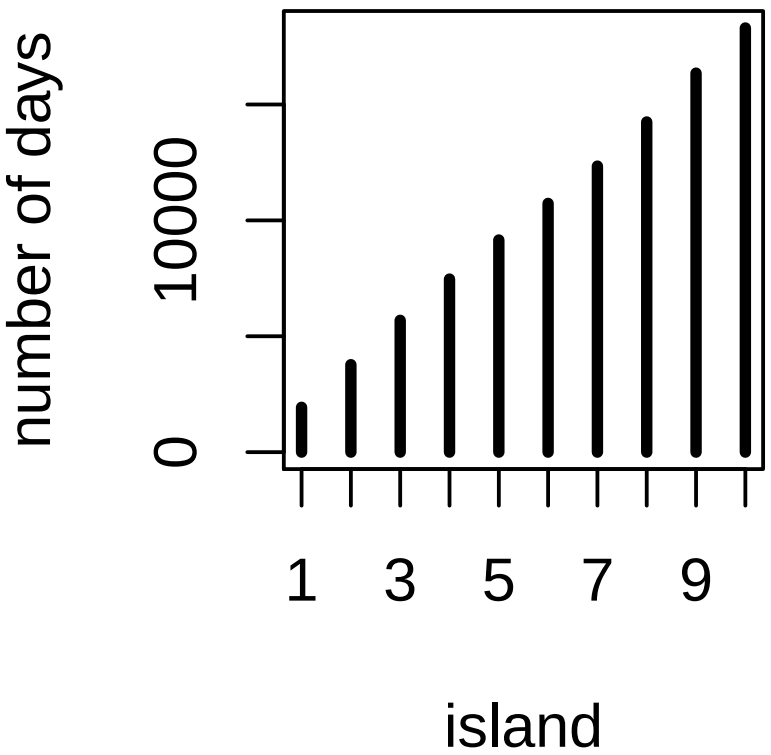
- So, if $P_{proposed} > P_{current}$, $P_{proposed}/P_{current} > 1$ and $p_{move} = 1$.
- For example, $current = 4$ and $proposed = 5$, $5/4 > 1$ so we move to the proposed island (with probability 1).
- On the other hand, if $P_{proposed} < P_{current}$, $P_{proposed}/P_{current} < 1$, and $p_{move} = P_{proposed}/P_{current}$.
- For example, $current = 4$ and $proposed = 3$, $3/4 < 1$ 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 Bernoulli distribution (Binomial with 1 trial) 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 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 θ, 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 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 θ.
- 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:

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

Why it works

- On the other hand, if we are presently at position $\theta + 1$, the probability of moving to θ is:

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

- The ratio of the transition probabilities is:

$$\frac{p(\theta \rightarrow \theta+1)}{p(\theta+1 \rightarrow \theta)} = \frac{0.5 \min\left(P(\theta+1)/P(\theta), 1\right)}{0.5 \min\left(P(\theta)/P(\theta+1), 1\right)}$$

$$= \begin{cases} \frac{1}{P(\theta)/P(\theta+1)} & \text{if } P(\theta+1) > P(\theta) \\ \frac{P(\theta+1)/P(\theta)}{1} & \text{if } P(\theta+1) < P(\theta) \end{cases}$$

$$= \frac{P(\theta+1)}{P(\theta)}$$

Why it works

- The last equation tells us that during transitions back and forth between adjacent positions, the relative probability of the transitions exactly matches the relative values of the target distribution.
- That might be enough to get the intuition that, in the long run, adjacent positions will be visited proportionally to their relative values in the target distribution.
- If that's true for adjacent positions, then, by extrapolating from one position to the next, it must be true for the whole range of positions.
- In more mathematical terms, this means that the transition probabilities form a Markov chain that has the target distribution as its equilibrium or stationary distribution. [Wikipedia, 2021]
- Hence, one can obtain a sample of the desired distribution by recording states from the chain.

The Metropolis Algorithm more Generally

- So far, we have only considered the case with a single discrete parameter θ that can only move to the left or right.
- The general Metropolis algorithm allows working with multiple continuous parameters $\theta_1, \theta_2, \ldots, \theta_n$ and more general proposal distributions.
- The essentials of the general method are the same as for the simple case.
- First, we have some target distribution $P(\theta)$ (θ can be a vector of parameters) from which we would like to generate representative sample values.
- We must be able to compute the value of $P(\theta)$ for any candidate value of θ.
- The distribution, $P(\theta)$, does not have to be normalized, however.
- Just needs needs to be nonnegative.

The Metropolis Algorithm more Generally

- In our Bayesian inference application $P(\theta)$ is the unnormalized posterior distribution on θ, which is the product of the likelihood and the prior: $f(d|\theta) * f(\theta)$.
- This is a very important property of MCMC, as it allows us to draw samples from the posterior without having to calculate the evidence $f(d)$.
- Sample values from the target distribution are generated by taking a random walk through the parameter space.
- Proposal distributions can take many different forms, the goal being to use a proposal distribution that efficiently explores the regions of the parameter space where $P(\theta)$ has most of its probability area.
- The generic case is using a Gaussian distribution centered at the current position.
- So the proposed move will typically be near the current position, with the probability of proposing a more distant position dropping off according to the normal curve.
- For multivariate target distributions, we can use a Multi-variate Gaussian to propose multi-dimensional points in each step.

Gibbs Sampling

- The Metropolis algorithm works whenever the probability of proposing a jump to B from A is equal to the probability of proposing A from B, when the proposal distribution is symmetric (such as a Gaussian distribution).
- There is a more general method, known as Metropolis-Hastings, that allows asymmetric proposals.
- This would mean, that the politician's coin were biased to lead him clockwise on average.
- Asymmetric proposal distributions allows us to explore the posterior distribution more efficiently (i.e., acquire a good image of the posterior distribution in fewer steps).
- Gibbs sampling is a variant of the Metropolis-Hastings algorithm that uses clever proposals and is therefore more efficient.
- The improvement arises from adaptive proposals in which the distribution of proposed parameter values adjusts itself intelligently, depending upon the parameter values at the moment.

Gibbs Sampling

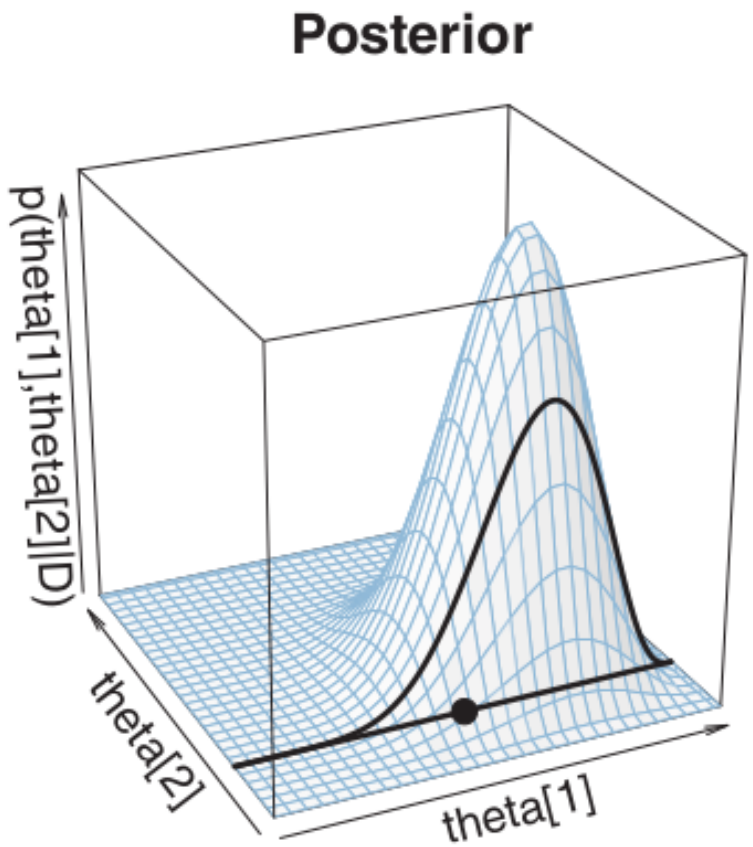
- How Gibbs sampling computes these adaptive proposals depends upon using conjugate combinations of priors and likelihoods (such as the Beta and the Binomial).
- As previously presented, conjugate combinations have analytical solutions for the posterior distribution of an individual parameter.
- And these solutions are what allow Gibbs sampling to make smart jumps around the joint posterior distribution of all parameters.
- The algorithm works as follows:
- At each point in the walk, the parameters are selected in an iterative cycle: $\theta_1, \theta_2, \theta_3, \ldots \theta_1, \theta_2, \theta_3, \ldots$.
- Suppose that parameter θ_i has been selected.
- Gibbs sampling then chooses a new value for that parameter by generating a random value directly from the conditional probability distribution of that parameter given all the others and d:

$$f(\theta_i|\theta_1, \ldots, \theta_{i-1}, \theta_{i+1}, \ldots, \theta_n, d)$$

Gibbs Sampling

- Since we are using conjugate combinations, this conditional distribution has a closed form that facilitates the sampling of random numbers from it.
- The new value for θ_i , combined with the unchanged values of $\theta_1, \ldots, \theta_{i-1}, \theta_{i+1}, \ldots, \theta_n$, constitutes the new position in the random walk.
- The process then repeats: select the next parameter θ_{i+1} and select a new value for that parameter from its conditional posterior distribution.
- Let's illustrate this process for a two-parameter example: θ_1, θ_2.
- In the first step, we want to select a new value for θ_1 .
- We conditionalize on the values of all the other parameters from the previous step in the chain.
- In this example, there is only one other parameter, namely θ_2.

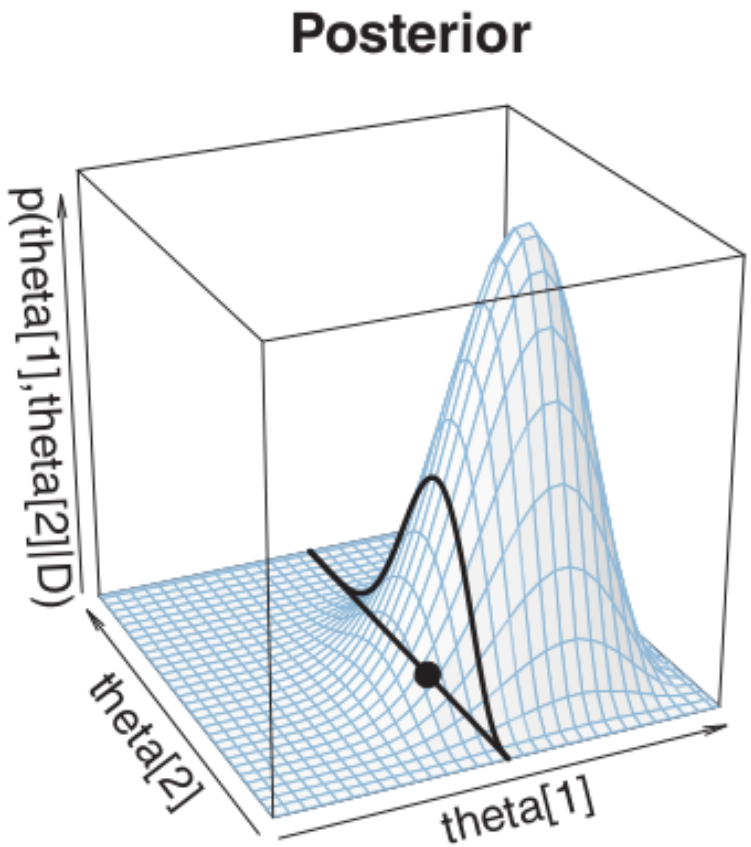
Gibbs Sampling



- The figure shows a slice through the joint distribution at the current value of θ_2.
- The heavy curve is the posterior distribution conditional on this value of θ_2, which is $f(\theta_1|\theta_2, d)$ in this case because there is only one other parameter.

Gibbs Sampling

- Because we are using conjugate distributions a computer can directly generate a random value of θ_1 from $f(\theta_1|\theta_2, d)$.
- Having generated a new value for θ_1, we then conditionalize on it and determine the conditional distribution of the next parameter, θ_2 using $f(\theta_2|\theta_1, d)$ as shown below:



- We generate a new value of θ_2 , and the cycle repeats.

Gibbs Sampling

- Because the proposal distribution exactly mirrors the posterior probability for that parameter, the proposed move is always accepted.
- Hence, the algorithm is more efficient than the standard Metropolis algorithm in which proposals are rejected in many cases.
- But there are some limitations to Gibbs sampling.
- First, there are cases when we don't want to use conjugate priors.
- Second, it can become inefficient with complex models containing hundreds, thousands or tens of thousands of parameters.

Hamiltonian Monte Carlo

- The Metropolis algorithm and Gibbs sampling are both highly random procedures.
- They try out new parameter values and see how good they are, compared to the current values.
- But Gibbs sampling gains efficiency by reducing this randomness and exploiting knowledge of the target distribution.
- Hamiltonian Monte Carlo (or Hybrid Monte Carlo, HMC) is another sampling method that is much more computationally costly than the others but its proposals are much more efficient.
- As a result, it doesn't need as many samples to describe the posterior distribution.
- And as models become more complex (thousands or tens of thousands of parameters) HMC can really outshine other algorithms.

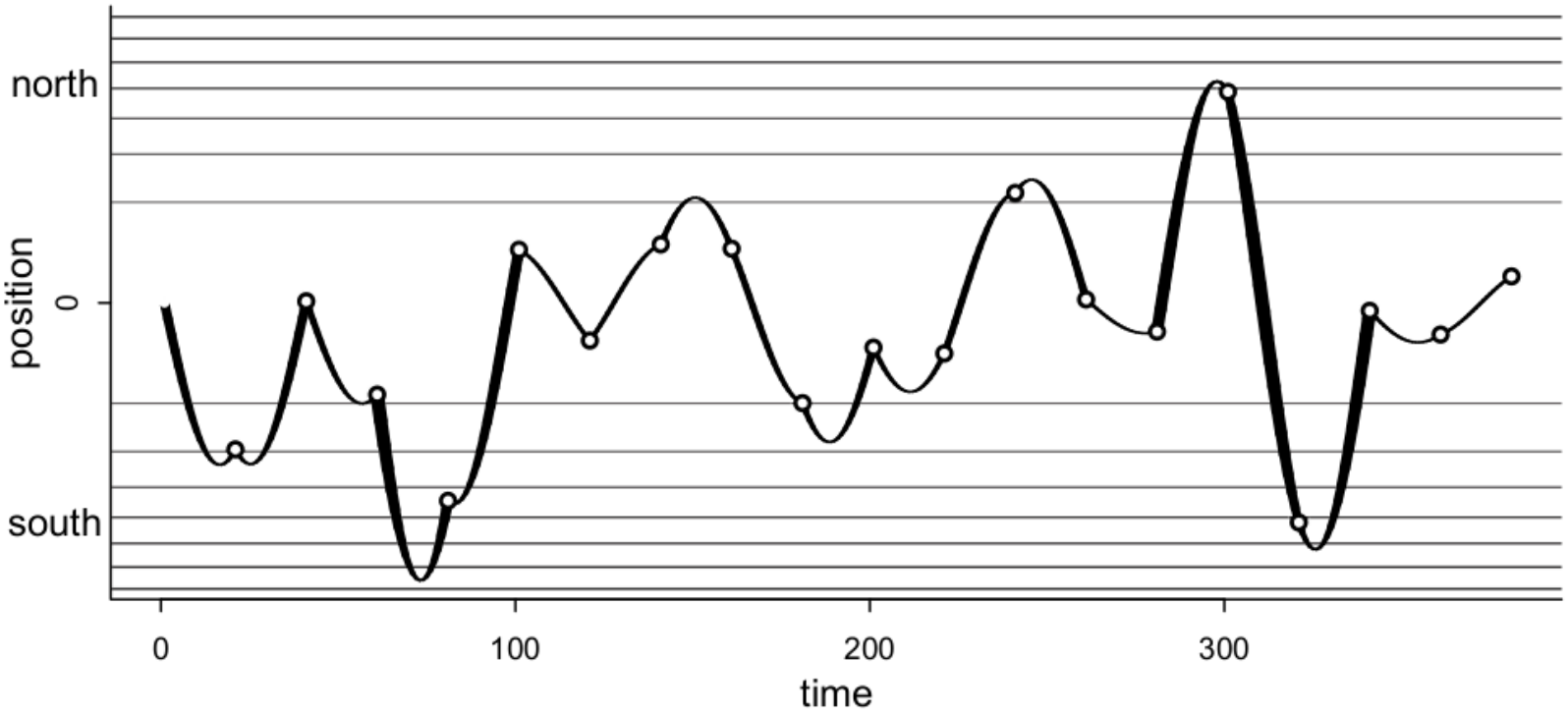
Hamiltonian Monte Carlo

- HMC is a very complex algorithm and we won't get into the details of its inner workings
- Let's try to understand it in a very superficial way by using again the politician's tale.
- Suppose the politician has moved to the mainland now.
- Now, instead of moving over a set of discrete islands, it has to move through a continuous territory stretched out along a narrow valley, running north-south.
- The obligations are the same: to visit his citizens in proportion to their local density.
- And again, the politician doesn't know the population of each area in advance.

Hamiltonian Monte Carlo

- The strategy of the politician is the following:
- He drives his car across the narrow valley back and forth along its length.
- In order to spend more time in densely settled areas, he slows down his vehicle when houses grow more dense.
- Likewise, he speeds up when houses grow more sparse.
- This strategy requires knowing how quickly population density is changing, at their current location.
- But it doesn't require remembering where they've been or knowing the population distribution anyplace else.
- This story is analogous to how Hamiltonian Monte Carlo works.

Hamiltonian Monte Carlo



Hamiltonian Monte Carlo

- In statistical applications, the politician's vehicle is the current vector of parameter values.
- HMC really does run a physics simulation, pretending the vector of parameters gives the position of a little frictionless particle.
- The log-posterior provides a surface for this particle to glide across.
- Then the job is to sweep across this surface, adjusting speed in proportion to how high up we are.
- When the log-posterior is very flat, then the particle can glide for a long time before the slope (gradient) makes it turn around.
- When instead the log-posterior is very steep, then the particle doesn't get far before turning around.

Hamiltonian Monte Carlo

- A big limitation of HMC is that it needs to be tuned to a particular model and its data.
- Stan[1] is a very popular platform for statistical modeling and high-performance statistical computation.
- Stan automates much of that tuning.
- Next, we will see how to use Stan to fit a linear model with an interaction.
- Make sure that the **rstan** package is installed to access Stan from within R.

[1] https://mc-stan.org/

Easy HMC: ulam

- Stan provides its own language to delcare models.
- The rethinking package provides a convenient interface, **ulam**, to compile lists of formulas, like the lists we've been using so far to construct quap estimates, into Stan HMC code.
- All that ulam does is translate formulas into Stan models, and then Stan defines the sampler and does the hard part.
- Stan models look very similar, but require some more explicit definitions.
- We will show them later.
- Before using ulam we must preprocess any variable transformations (log, exp, etc).
- We also must construct a clean data list with only the variables we will use.

A model of ruggedness

- We are are going to work with the **rugged** dataset from the rethinking package.
- Each row in these data is a country, and the various columns are economic, geographic, and historical features.
- The variable rugged is a Terrain Ruggedness Index that quantifies the topographic heterogeneity of a landscape.
- The outcome variable of our regression model will be the logarithm of real gross domestic product per capita, from the year 2000, **rgdppc_2000**.
- Ruggedness is usually associated with poorer countries, in most of the world.
- Rugged terrain usually means transport is difficult, which means market access is hampered, which means reduced gross domestic product.
- However, this associated gets inverted for African countries.

A model of ruggedness

- Let's load and explore the data:

```
library(rethinking)
data(rugged)
d <- rugged
d$log_gdp <- log(d$rgdppc_2000)
#remove rows with missing values
dd <- d[ complete.cases(d$rgdppc_2000) , ]
# discard columns we are not going to use
dd.trim <- dd[ , c("log_gdp","rugged","cont_africa") ]
summary(dd.trim)
```

```
> summary(dd.trim)
    log_gdp          rugged        cont_africa
 Min.   : 6.146   Min.   :0.0030   Min.   :0.0000
 1st Qu.: 7.539   1st Qu.:0.4422   1st Qu.:0.0000
 Median : 8.578   Median :0.9795   Median :0.0000
 Mean   : 8.517   Mean   :1.3332   Mean   :0.2882
 3rd Qu.: 9.480   3rd Qu.:1.9572   3rd Qu.:1.0000
 Max.   :10.965   Max.   :6.2020   Max.   :1.0000
```

A model of ruggedness

- Let's load and explore the data:

```
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#remove rows with missing values
dd <- d[ complete.cases(d$rgdppc_2000) , ]
# discard columns we are not going to use
dd.trim <- dd[ , c("log_gdp","rugged","cont_africa") ]
# convert cont_africa to factor
dd.trim$cont_africa<-as.factor(dd.trim$cont_africa)
```

```
> summary(dd.trim)
    log_gdp          rugged       cont_africa
 Min.   : 6.146   Min.   :0.0030   0:121
 1st Qu.: 7.539   1st Qu.:0.4422   1: 49
 Median : 8.578   Median :0.9795
 Mean   : 8.517   Mean   :1.3332
 3rd Qu.: 9.480   3rd Qu.:1.9572
 Max.   :10.965   Max.   :6.2020
```

A model of ruggedness

- We have a dataset with countries as rows and 3 columns:
  1. log_gdp: the log GDP of the country in year 2000.
  2. rugged: the Terrain Ruggedness Index of the country
  3. cont_africa: a binary variable (1 for African countries and 0 for non-African ones).
- Let's compute the correlation between log_gdp and rugged:

```
> cor(dd.trim$rugged,dd.trim$log_gdp)
[1] 0.002833496
```

- It is very low. Now let's calculate them separately for African and non-African countries:

```
> dd.A<-dd.trim[dd.trim$cont_africa==1,]
> cor(dd.A$rugged,dd.A$log_gdp)
[1] 0.2607532
>
> dd.NA<-dd.trim[dd.trim$cont_africa==0,]
> cor(dd.NA$rugged,dd.NA$log_gdp)
[1] -0.2307945
```

- We now observe a stronger relationship between the two variables that is reversed for African and non-African countries.

A model of ruggedness

- We will now construct a Bayesian Linear Regression between log GDP (y) and terrain ruggedness (x) capable of incorporating the different relationships for these two groups of countries encoded by the variable A.
- As we learned in a previous lecture, interactions are a convenient way to include different slopes for different categories in our data.
- Our model will be as follows:

$$
\begin{aligned}
y_i &\sim N(\mu_i, \sigma) && \text{[likelihood]} \\
\mu_i &= \beta_0 + \beta_1 x_i + \beta_2 A_i + \beta_3 * x_i * A_i && \text{[linear model]} \\
\beta_0 &\sim N(0, 100) && [\beta_0 \text{ prior}] \\
\beta_1 &\sim N(0, 10) && [\beta_1 \text{ prior}] \\
\beta_2 &\sim N(0, 10) && [\beta_2 \text{ prior}] \\
\beta_3 &\sim N(0, 10) && [\beta_3 \text{ prior}] \\
\sigma &\sim \text{Cauchy}(0, 2) && [\sigma \text{ prior}]
\end{aligned}
$$

- We put Gaussian priors on all β coefficients and a Cauchy prior for σ (a t-student with 1 degree of freedom).
- The Cauchy distribution is heavy-tailed and has proven to be a useful prior for standard deviations (especially when restrained to postive values, taking the name of half-Cauchy).

A model of ruggedness

- The R code for the model would be:

```
model<-alist(
  log_gdp ~ dnorm( mu , sigma ) ,
  mu <- b0 + b1*rugged + b2*cont_africa
  + b3*rugged*cont_africa,
  b0 ~ dnorm(0,100),
  b1 ~ dnorm(0,10),
  b2 ~ dnorm(0,10),
  b3 ~ dnorm(0,10),
  sigma ~ dcauchy(0,2)
)
```

Conclusions

- This class has been an introduction to Markov chain Monte Carlo (MCMC) estimation.
- The goal has been to introduce the purpose and approach MCMC algorithms.
- The major algorithms introduced were the Metropolis, Gibbs sampling, and Hamiltonian Monte Carlo algorithms.
- Each has its advantages and disadvantages.
- A function in the rethinking package, ulam , was introduced that uses the Stan Hamiltonian Monte Carlo engine to a linear model with an interaction.

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