Markov Chain Monte Carlo

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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.
- This class is based on Chapter 9 of [McElreath, 2020] and Chapter 7 of [Kruschke, 2014].

Markov Chain Monte Carlo

- More advanced models such as generalized 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.
- 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.

Markov Chain Monte Carlo

- 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 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 $\mathbb{P}_{move} = P_{proposed}/P_{current}$.
- 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.
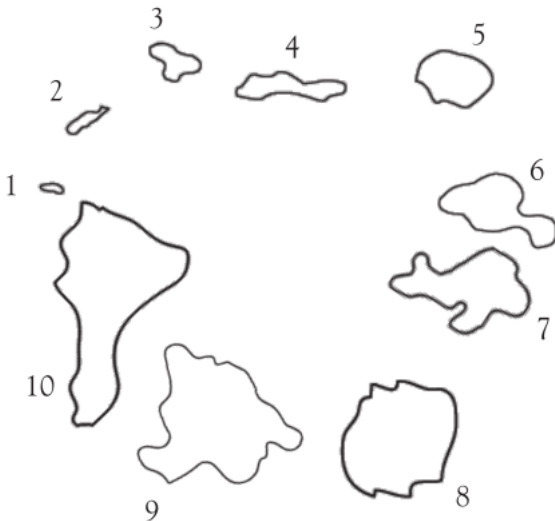
The Metropolis algorithm

- 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.

$$\mathbb{P}_{move} = \min(1, P_{proposed}/P_{current}). \tag{1}$$

- So, if $P_{proposed} > P_{current}$, $P_{proposed}/P_{current} > 1$ and $\mathbb{P}_{move} = 1$.
- 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 $\mathbb{P}_{move} = P_{proposed}/P_{current}$.
- 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")
```
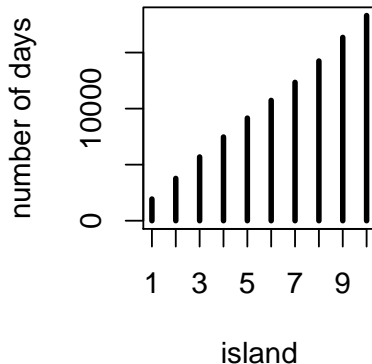
The time spent on each island is proportional to its population size.

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 coin flip represents the **proposal distribution** $q(\theta)$, which for continuous parameters is usually replaced by a Gaussian 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.
- We are going to denote our target probability density from which we want to draw samples as $p(\theta)$.
- Bear in mind that $p(\theta)$ is usually a posterior density $f(\theta|d)$.
- 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 density $p(\theta)$.
- 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.

Why it works

- The probability of moving to $\theta + 1$, denoted $\mathbb{P}(\theta \to \theta + 1)$, is the probability of proposing that move times the probability of accepting it if proposed, which is:

$$\mathbb{P}(\theta \to \theta + 1) = 0.5 \times \min(p(\theta + 1)/p(\theta), 1)$$

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

$$\mathbb{P}(\theta + 1 \to \theta) = 0.5 \times \min(p(\theta)/p(\theta + 1), 1)$$

- The ratio of the transition probabilities is:

$$\frac{\mathbb{P}(\theta \to \theta + 1)}{\mathbb{P}(\theta + 1 \to \theta)} = \frac{0.5 \times \min(p(\theta + 1)/p(\theta), 1)}{0.5 \times \min(p(\theta)/p(\theta + 1), 1)} \tag{2}$$

$$= \begin{cases} \frac{1}{p(\theta)/p(\theta+1)} & \text{if} p(\theta + 1) > p(\theta) \\ \\ \frac{p(\theta+1)/p(\theta)}{1} & \text{if} p(\theta + 1) < p(\theta) \end{cases} \tag{3}$$

$$= \frac{p(\theta + 1)}{p(\theta)} \tag{4}$$

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 $\vec{\theta} = \{\theta_1, \theta_2, \ldots, \theta_m\}$ and more general proposal distributions.
- The essentials of the general method are the same as for the simple case.
- First, we have some target density $p(\theta)$ (θ can be a vector of parameters $\vec{\theta}$) from which we would like to generate representative sample values:

$$\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(j)}, \ldots, \theta^{(k)}$$

- Note that each parameter sample $\theta^{(j)}$ can be a multidimensional vector $\vec{\theta}^{(j)}$ if we have multiple parameters.
- We must be able to compute the value of $p(\theta)$ for any candidate value of θ.
- The density $p(\theta)$, 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 density 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 $\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(k)}$ are generated by taking a random walk through the parameter space.
- The proposal distribution $q(\theta)$ aims to explore $p(\theta)$ allowing us to visit any parameter value on the continuum.
- The proposals from $q(\theta)$ should go a reasonable distance in the parameter space (otherwise the random walk moves too slowly).
- They should also not be rejected too frequently (otherwise the random walk wastes too much time standing still) [Gelman et al., 2013].

- The generic case for $q(\theta)$ is using a Gaussian distribution centered at the current position $\theta^{(t-1)}$.

$$q(\theta^{(t)}|\theta^{(t-1)}) = N(\theta^{(t-1)}, \sigma^2)$$

where σ is a user-specified parameter.

- 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 $p(\vec{\theta})$, we can use a Multi-variate Gaussian to propose multi-dimensional points in each step.

$$q(\vec{\theta}^{(t)}|\vec{\theta}^{(t-1)}) = N(\vec{\theta}^{(t-1)}, \Sigma)$$

The Metropolis Algorithm more Generally

- A general form of the Metropolis algorithm as described in [Gelman et al., 2013] is given below:

The Metropolis Algorithm

1. Draw a starting point θ^0 for which $p(\theta^0) > 0$.

2. For $t = 1, 2, \ldots, k$:

   1. Sample a proposal θ^* from the proposal distribution at time t: $q(\theta^*|\theta^{(t-1)})$
   2. Calculate the ratio of the densities:

   $$r = \frac{p(\theta^*)}{p(\theta^{t-1})} \tag{5}$$

   3. Set

   $$\theta^{(t)} = \begin{cases} \theta^* & \text{with probability } \min(r, 1) \\ \theta^{(t-1)} & \text{otherwise} \end{cases} \tag{6}$$

   4. Return $\theta^{(1)}, \ldots, \theta^{(k)}$.

If the proposed value θ^* happens to land outside the permissible bounds of θ (e.g., when $0 \leq \theta \leq 1$), $p(\theta^*)$ is set to zero, hence $\theta^{(t)} = \theta^{(t-1)}$.

The Metropolis-Hastings Algorithm

- 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).

$$q(\theta^{(a)}|\theta^{(b)}) = q(\theta^{(b)}|\theta^{(a)})$$

- We cam easisly check this using R:

```
> a<-0.5
> b<-0.3
> dnorm(x=a,mean=b)
[1] 0.3910427
> dnorm(x=b,mean=a)
[1] 0.3910427
```

- There is a more general method, known as Metropolis-Hastings, that allows asymmetric proposals (i.e., $q(\theta^{(a)}|\theta^{(b)}) \neq q(\theta^{(b)}|\theta^{(a)})$).
- This would mean, that the politician's coin were biased to lead him clockwise on average.

The Metropolis-Hastings Algorithm

- To correct for the asymmetry in the proposals, the ratio r in Equation 5 is replaced by a ratio of ratios:

$$r = \frac{p(\theta^*)/q(\theta^*|\theta^{(t-1)})}{p(\theta^{t-1})/q(\theta^{(t-1)}|\theta^*)} \tag{7}$$

- 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).
- The goal is that regions with high probability density in $p(\theta)$ to be proposed more frequently than regions with low probability density.
- The ideal proposal distribution $q(\theta^*|\theta^{(t-1)})$ would be the target distribution $p(\theta^*)$.
- Then the ratio r in Equation 7 is always exactly 1.
- However, in practical settings is not possible so sample directly from $p(\theta^*)$, which indeed is the reason why we use MCMC methods.

Gibbs Sampling

- 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.
- 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.

Gibbs Sampling

- The algorithm works as follows:
- First, we assume that our target parameter θ is multi-dimensional: $\vec{\theta} = \{\theta_1, \theta_2, \ldots, \theta_m\}$
- 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_j 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:

$$q(\theta_j^* | \theta^{(t-1)}) = p(\theta_j^* | \theta_{-j}^{(t-1)}) = p(\theta_j^* | \theta_1^{(t-1)}, \ldots, \theta_{j-1}^{(t-1)}, \theta_{j+1}^{(t-1)}, \ldots, \theta_m^{(t-1)})$$

- Since we are using conjugate combinations, this conditional distribution has a closed form that facilitates the sampling of random numbers from it.

Gibbs Sampling

- The new value for $\theta_j^{(t)}$, combined with the unchanged values of $\theta_1^{(t-1)}, \ldots, \theta_{j-1}^{(t-1)}, \theta_{j+1}^{(t-1)}, \ldots, \theta_m^{(t-1)}$, constitutes the new position in the random walk.

$$\{\theta_1^{(t)}, \ldots, \theta_{j-1}^{(t)}, \theta_j^{(t)}, \theta_{j+1}^{(t)}, \ldots, \theta_m^{(t)}\} = \{\theta_1^{(t-1)}, \ldots, \theta_{j-1}^{(t-1)}, q(\theta_j^* | \theta^{(t-1)}), \theta_{j+1}^{(t-1)}, \ldots, \theta_m^{(t-1)}\}$$

- The process then repeats: select the next parameter θ_{j+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 $\theta_1^{(t)}$.
- 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.
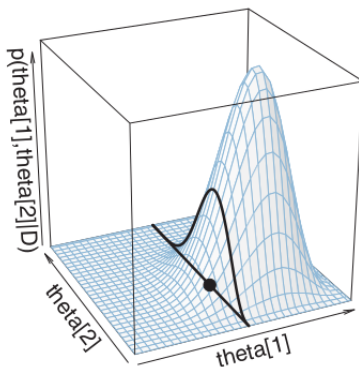
Gibbs Sampling

Posterior
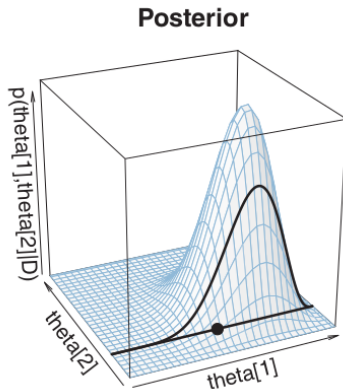
- The figure shows a slice through the target joint distribution $p(\theta)$ at the current value of $\theta_2^{(t-1)}$.
- The heavy curve is the target distribution conditional on this value of $\theta_2^{(t-1)}$.
- This corresponds to $p(\theta_1 | \theta_2^{(t-1)})$ in this case because there is only one other parameter.

Gibbs Sampling

- Because we are using conjugate distributions a computer can directly generate a random value of $\theta_1^{(t)}$ from $p(\theta_1|\theta_2^{(t-1)})$.

- Having generated $\theta_1^{(t)}$, we then conditionalize on it and determine the conditional distribution of the next parameter, $\theta_2^{(t+1)}$ using $p(\theta_2|\theta_1^{(t)})$ as shown below:

Posterior

- We generate a new value $\theta_2^{(t+1)}$, and the cycle repeats.

Gibbs Sampling

- Because the proposal distribution exactly mirrors the posterior probability for that parameter, the proposed move is always accepted.
- The proof of this can be found on page on page 281 of [Gelman et al., 2013], but essentially since $q(\theta_j^* | \theta^{(t-1)}) = p(\theta_j^* | \theta_{-j}^{(t-1)})$, the ratio r from Equation 7 becomes 1.
- 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.
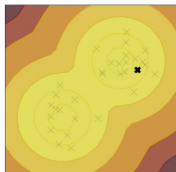- This story is analogous to how Hamiltonian Monte Carlo works.

Hamiltonian Monte Carlo

- 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 (momentum) 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.
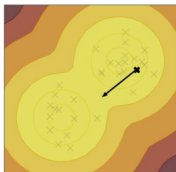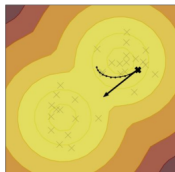
Hamiltonian Monte Carlo
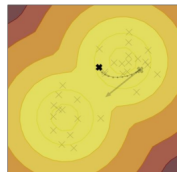
start at prev. sample   random momentum   simulate dynamics   accept / reject

source: [Izmailov et al., 2021]

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.

Stan

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

- 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 association is not valid 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
```

- Note that we do not convert cont_africa into a factor because that produces numerical problems with the rethinking methods.

A model of ruggedness

- We end up with a data.frame formed by the countries as rows and the following 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:

```r
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)
)
```

- Let's try to fit this model using Laplace Approximation:

```r
> b.reg3<-quap(model,data=dd.trim)
Error in quap(model, data = dd.trim) :
  initial value in 'vmmin' is not finite
The start values for the parameters were invalid.
```

- The optimizer is having a hard time finding the MAP estimates for this model!
- This can sometimes be corrected by using start values (declared with the **start** parameter), but in many models even this does not help.

A model of ruggedness

- After trying to fit b.reg3 with quap many times, it worked!

```
> precis(b.reg3)
        mean   sd  2.5% 97.5%
b0      9.22 0.14  8.95  9.49
b1     -0.20 0.08 -0.35 -0.05
b2     -1.95 0.22 -2.39 -1.51
b3      0.39 0.13  0.14  0.65
sigma   0.93 0.05  0.83  1.03
```

- Let's interpret the mean values for the posterior marginals of each β coefficient:
  - mean(b0) = 9.22: this is the intercept for non-African countries.
  - mean(b1)=-0.20: this is the slope for non-African countries, which is clearly negative.
  - mean(b2)=-1.95: this is the difference between the intercept for African and non-African countries, which indicates that African countries have a lower GDP than non-African countries when rugedness is zero $(9.22 - 1.95 = 7.27)$
  - mean(b3)=0.39: this is the difference between the slopes for African and non-African countries, which indicates that the slope for African countries is positive $(-0.2 + 0.39 = 0.19)$.

Ulam

- Now, let's fit the same model using Stan HMC with **ulam**:

  ```
  m.reg1 <- ulam(model ,data=dd.trim)
  ```

- After messages about compiling, and sampling, ulam returns an object that contains a bunch of summary information, as well as samples from the posterior distribution.

- This process takes much longer than **quap**.

- We can summarize just like with quap:

  ```
  > precis(m.reg1, prob=0.95 )
          mean   sd  2.5% 97.5% n_eff Rhat4
  b0      9.21 0.15  8.89  9.51   169  1.03
  b1     -0.20 0.09 -0.37 -0.01   163  1.04
  b2     -1.95 0.23 -2.37 -1.48   241  1.01
  b3      0.39 0.13  0.10  0.66   243  1.03
  sigma   0.95 0.05  0.85  1.06   348  1.00
  ```

- These estimates are very similar to the Laplace approximation.

Ulam

- A report of the chain can be obtained with command **show**:

```
> show(m.reg1)
Hamiltonian Monte Carlo approximation
500 samples from 1 chain

Sampling durations (seconds):
        warmup sample total
chain:1    0.2   0.17   0.37

Formula:
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)
```

Stan Code

We can also get the Stan code with: `stancode(m.reg1)`:

```
data{
    vector[170] log_gdp;
    int cont_africa[170];
    vector[170] rugged;
}
parameters{
    real b0;
    real b1;
    real b2;
    real b3;
    real sigma;
}
```

```
model{
    vector[170] mu;
    sigma ~ cauchy( 0 , 2 );
    b3 ~ normal( 0 , 10 );
    b2 ~ normal( 0 , 10 );
    b1 ~ normal( 0 , 10 );
    b0 ~ normal( 0 , 100 );
    for ( i in 1:170 ) {
        mu[i] = b0 + b1 * rugged[i] + b2 * cont_africa[i]
        + b3 * rugged[i] * cont_africa[i];
    }
    log_gdp ~ normal( mu , sigma );
}
```

This is Stan code, not R code. It is essentially the formula list we provided to ulam, but in reverse order.

Additional Ulam Parameters

- **iter**: the number of samples from the chain. The default is 1000.
- **warmup**: the number of tuning samples. These samples are used to adapt sampling, and so are not actually part of the target posterior distribution. The default value is iter/2 , which gives us 500 warmup samples and 500 real samples to use for inference.
- **chains**: the number of independent Markov chains to sample from. All of the non-warmup samples from each chain will be automatically combined in the resulting inferences.
- **cores**: the number of procesors over which the chains will be distributed.

Ulam

- Let's fit the same model sampling 4 different chains distributed over 4 CPU cores with 3000 iterarions and 1000 warmups.

```
> m.reg2 <- ulam(model ,data=dd.trim, iter=3000,
               warmup =1000, chains=4, cores=4)
> show(m.reg2)
Hamiltonian Monte Carlo approximation
8000 samples from 4 chains

Sampling durations (seconds):
        warmup sample total
chain:1   0.62   1.08   1.70
chain:2   0.54   1.06   1.60
chain:3   0.60   0.89   1.49
chain:4   0.37   0.82   1.19
```

Diagnostic criteria: n_eff and Rhat

- Note that **precis** reported two new columns: n_eff and Rhat, which provide MCMC diagnostic criteria.
- They help us tell how well estimation worked.
- The column n_eff is a crude estimate of the number of independent samples we managed to get.
- When n_eff is much lower than the actual number of iterations (minus warmup) of your chains, it means the chains are inefficient, but possibly still okay.
- Rhat is the Gelman Rubin convergence diagnostic, which estimates the convergence of the Markov chains to the target distribution.
- It should approach 1.00 from above, when all is well.
- When Rhat is above 1.00, it usually indicates that the chain has not yet converged, and probably we shouldn't trust the samples.
- If we draw more iterations, it could be fine, or it could never converge.

Ulam

- We can extract samples from the posterior in the usual way:

  `post <- extract.samples( m.reg1 )`
- We also use **link** and **sim** functions to get posterior predictions.
- We can plot the correlations between samples using the function **pairs**:

  `pairs( m.reg1)`
- This will show a pairs plot: a matrix of bivariate scatter plots.
- Along the diagonal the smoothed histogram of each parameter is shown, along with its name.
- In in the lower triangle of the matrix, below the diagonal, the correlation between each pair of parameters is shown, with stronger correlations indicated by relative size.

Ulam Pairs
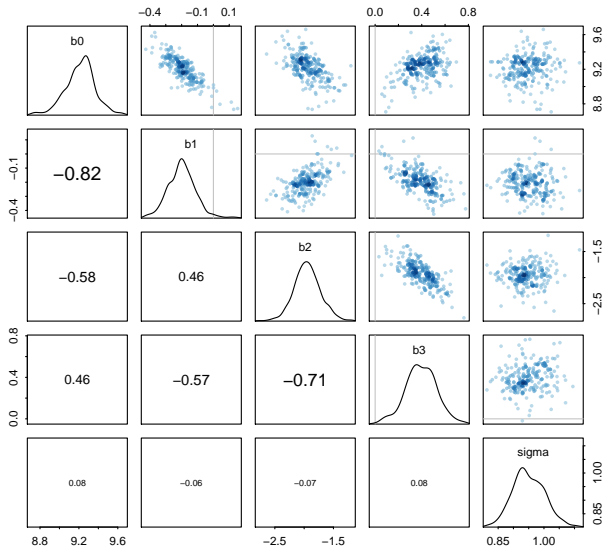
- For this model and these data, the resulting posterior distribution is quite nearly multivariate Gaussian.
- The density for sigma is certainly skewed in the expected direction.
- But otherwise the Laplace approximation does almost as well as Hamiltonian Monte Carlo.
- This is a very simple kind of model structure of course, with Gaussian priors, so an approximately Gaussian posterior should be no surprise.
- For more complex models, posterior distributions can take more exotic shapes.

Checking the Chain

- If the Markov chain is defined correctly then it is guaranteed to converge in the long run to the right posterior distribution.
- But the machine can sometimes fail.
- We won't study these cases in detail.
- A trace plot is a very useful tool for diagnosing malfunction.
- It basically plots the samples in sequential order, joined by a line.
- In the terrain ruggedness example, the trace plot shows a very healthy chain.
- We can obtain it with the following command:

```
traceplot( m.reg1 )
```
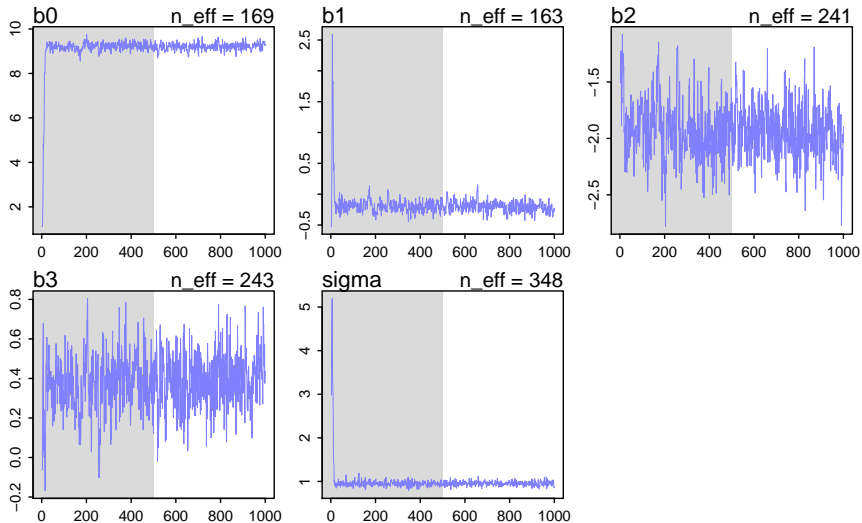
Checking the Chain

- The plot shows the zig-zagging trace of each parameter as the path the chain took through each dimension of parameter space.
- The gray region in each plot, the first 500 samples, marks the warmups samples.
- During adaptation, the Markov chain is learning to more efficiently sample from the posterior distribution.
- So these samples are not necessarily reliable to use for inference.
- They are automatically discarded by **extract.samples**, which returns only the samples shown in the white regions.
- Typically we look for two things in these trace plots: stationarity and good mixing.

Checking the Chain

- Stationarity refers to the path staying within the posterior distribution.
- Notice that these traces, all stick around a very stable central tendency.
- Another way to think of this is that the mean value of the chain is quite stable from beginning to end.
- A well-mixing chain means that each successive sample within each parameter is not highly correlated with the sample before it, which is known as **autocorrelation**.
- Visually, we can see this by the rapid zig-zag motion of each path, as the trace traverses the posterior distribution without getting mired anyplace.

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 fit a linear model with an interaction.

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