08: Markov chain Monte Carlo

Statistical Rethinking













Drawing the Bayesian Owl

- 1. Theoretical estimand
- 2. Scientific (causal) model(s)
- 3. Use 1 & 2 to build statistical model(s)
- 4. Simulate from 2 to validate 3 yields 1
- 5. Analyze real data



aNAlYzE rEAl DatA





Computing the posterior

- 1. Analytical approach (often impossible)
- 2. Grid approximation (very intensive)
- 3. Quadratic approximation (limited)
- 4. Markov chain Monte Carlo (intensive)





The Metropolis Archipelago









Contract: King Markov must visit each island in proportion to its population size







Here's how he does it...









(1) Flip a coin to choose island on left or right.Call it the "proposal" island.

Call it the "proposal" island.















3

(1) Flip a coin to choose island on left or right.

(2) Find population of proposal island.

 p_5

Call it the "proposal" island. (2) Find population of proposal island.

















(3) Find population of current island.







- (1) Flip a coin to choose island on left or right.

Call it the "proposal" island. (2) Find population of proposal island. (3) Find population of current island.













3

(4) Move to proposal, with probability = $\frac{p_5}{p_4}$





- (1) Flip a coin to choose island on left or right.

Call it the "proposal" island. (2) Find population of proposal island. (3) Find population of current island.





- (1) Flip a coin to choose island on left or right.
- (4) Move to proposal, with probability = $\frac{p_5}{2}$ p_4

(5) Repeat from (1)







3





(3) Find population of current island.

(5) Repeat from (1)

(2) Find population of proposal island.

- (1) Flip a coin to choose island on left or right. Call it the "proposal" island.
- (4) Move to proposal, with probability = $\frac{p_5}{2}$ p_4

This procedure ensures visiting each island in proportion to its population, in the long run.









Markov chain Monte Carlo

Usual use: Draw samples from a posterior distribution

"Islands": parameter values

"Population size": posterior probability

Visit each parameter value in proportion to its posterior probability

Any number of dimensions (parameters)





"Markov chain Monte Carlo"



Chain: Sequence of draws from distribution

Markov chain: History doesn't matter, just where you are now

Monte Carlo: Random simulation

30

40





Metropolis algorithm: Simple version of Markov chain Monte Carlo (MCMC)

Easy to write, very general, often inefficient

1	1	1
150	200	250



Metropolis, Rosenbluth, Rosenbluth, Teller and Teller (1953)

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER, Los Alamos Scientific Laboratory, Los Alamos, New Mexico

> EDWARD TELLER,* Department of Physics, University of Chicago, Chicago, Illinois (Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

AND





Metropolis, Rosenbluth, Rosenbluth, Teller and Teller (1953)

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state and to a four-term virial coefficient expansion.

to the free volume equation of state and to a four-term virial coefficient expansion.

- Equation of state calculations by fast computing machines
- ..., AW Rosenbluth, MN Rosenbluth... The journal of ..., 1953 aip.scitation.org
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Whirling Arcs of Steel!

Touche! Miss Arianna Wright, state women's champion and city champ in the men's foil tournaments, makes a deep and effective lunge to score a point against Vernon Bordman, who wields a good blade himself.

Arianna Rosenbluth (1927 - 2020)









MANIAC: Mathematical Analyzer, Numerical Integrator, and Computer

MANIAC: 1000 pounds 5 kilobytes of memory 70k multiplications/sec

Your laptop: 4–7 pounds 8+ million kilobytes memory Billions of multiplications/sec

MCMC is diverse

Metropolis has yielded to newer, more efficient algorithms

Many innovations in the last decades

Best methods use *gradients*

We'll use Hamiltonian Monte Carlo

Chapman & Hall/CRC Handbooks of Modern **Statistical Methods**

Handbook of Markov Chain Monte Carlo

Edited by **Steve Brooks** Andrew Gelman Galin L. Jones Xiao-Li Meng





Basic Rosenbluth (aka Metropolis) algorithm



Basic Rosenbluth (aka Metropolis) algorithm





Low probability

1.

High probability



and a



Hamiltonian Monte Carlo



Hamiltonian Monte Carlo







Pages 276–278

Overthinking: Hamiltonian Monte Carlo in the raw. The HMC algorithm needs five things to go: (1) a function U that returns the negative log-probability of the data at the current position (parameter values), (2) a function grad_U that returns the *gradient* of the negative log-probability at the current position, (3) a step size epsilon, (4) a count of leapfrog steps L, and (5) a starting position current_q. Keep in mind that the position is a vector of parameter values and that the gradient also needs to return a vector of the same length. So that these U and grad_U functions make more sense, let's present them first, built custom for the 2D Gaussian example. The U function just expresses the logposterior, as stated before in the main text:

$$\sum_{i} \log p(y_i | \mu_y, 1) + \sum_{i} \log p(x_i | \mu_x, 1) + \log p(\mu_y | 0)$$

So it's just four calls to dnorm really:

```
R code
        # U needs to return neg-log-probability
        U <- function( q , a=0 , b=1 , k=0 , d=1 ) {
            muy <- q[1]
            mux <- q[2]
            U <- sum( dnorm(y,muy,1,log=TRUE) ) + sum( dnorm(x,mux,1,log=TRUE) ) +</pre>
                dnorm(muy,a,b,log=TRUE) + dnorm(mux,k,d,log=TRUE)
            return( -U )
```

Now the gradient function requires two partial derivatives. Luckily, Gaussian derivatives are very clean. The derivative of the logarithm of any univariate Gaussian with mean a and standard deviation *b* with respect to *a* is:

$$\frac{\partial \log N(y|a,b)}{\partial a} = \frac{y-a}{b^2}$$

And since the derivative of a sum is a sum of derivatives, this is all we need to write the gradients:

$$\frac{\partial U}{\partial \mu_x} = \frac{\partial \log N(x|\mu_x, 1)}{\partial \mu_x} + \frac{\partial \log N(\mu_x|0, 0.5)}{\partial \mu_x} = 2$$

And the gradient for μ_{y} has the same form. Now in code form:

```
R code
```

```
# gradient function
# need vector of partial derivatives of U with respect to vector q
U_gradient <- function(q, a=0, b=1, k=0, d=1) {
    muy <- q[1]
    mux <- q[2]
    G1 <- sum(y - muy) + (a - muy)/b^2 #dU/dmuy
    G2 \leq sum(x - mux) + (k - mux)/d^2 #dU/dmux
    return( c( -G1 , -G2 ) ) # negative bc energy is neg-log-prob
# test data
set.seed(7)
y < - rnorm(50)
x < - rnorm(50)
x <- as.numeric(scale(x))</pre>
y <- as.numeric(scale(y))</pre>
```

The gradient function above isn't too bad for this model. But it can be terrifying for a reasonably complex model. That is why tools like Stan build the gradients dynamically, using the model definition. Now we are ready to visit the heart. To understand some of the details here, you should read Radford Neal's chapter in the Handbook of Markov Chain Monte Carlo. Armed with the log-posterior and gradient functions, here's the code to produce FIGURE 9.6:

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 $(0, 0.5) + \log p(\mu_x, 0, 0.5)$

```
\sum \frac{x_i - \mu_x}{1^2} + \frac{0 - \mu_x}{0.5^2}
```

```
library(shape) # for fancy arrows
Q <- list()
Q$q <- c(-0.1, 0.2)
pr <- 0.3
plot( NULL , ylab="muy" , xlab="mux" , xlim=c(-pr,pr) , ylim=c(-pr,pr) )
step <- 0.03
L <- 11 # 0.03/28 for U-turns --- 11 for working example
n_samples <- 4
path_col <- col.alpha("black",0.5)</pre>
points( Q$q[1] , Q$q[2] , pch=4 , col="black" )
for ( i in 1:n_samples ) {
    Q <- HMC2( U , U_gradient , step , L , Q$q )
    if ( n_samples < 10 ) {
      for ( j in 1:L ) {
        K0 <- sum(Q$ptraj[j,]^2)/2 # kinetic energy</pre>
        lines( Q$traj[j:(j+1),1] , Q$traj[j:(j+1),2] , col=path_col , lwd=1+2*K0 )
     points( Q$traj[1:L+1,] , pch=16 , col="white" , cex=0.35 )
     Arrows( Q$traj[L,1] , Q$traj[L,2] , Q$traj[L+1,1] , Q$traj[L+1,2] ,
          arr.length=0.35, arr.adj = 0.7)
     text( Q$traj[L+1,1] , Q$traj[L+1,2] , i , cex=0.8 , pos=4 , offset=0.4 )
    points( Q$traj[L+1,1] , Q$traj[L+1,2] , pch=ifelse( Q$accept==1 , 16 , 1 ) ,
        col=ifelse( abs(Q$dH)>0.1 , "red" , "black" ) )
```

The function HMC2 is built into rethinking. It is based upon one of Radford Neal's example scripts.¹⁵³ It isn't actually too complicated. Let's tour through it, one step at a time, to take the magic away. This function runs a single trajectory, and so produces a single sample. You need to use it repeatedly to build a chain. That's what the loop above does. The first chunk of the function chooses random momentum—the flick of the particle—and initializes the trajectory.

```
HMC2 <- function (U, grad_U, epsilon, L, current_q) {
 q = current_q
 p = rnorm(length(q), 0, 1) \# random flick - p is momentum.
 current_p = p
 # Make a half step for momentum at the beginning
 p = p - epsilon * grad_U(q) / 2
 # initialize bookkeeping - saves trajectory
 qtraj <- matrix(NA,nrow=L+1,ncol=length(q))</pre>
 ptraj <- qtraj
 qtraj[1,] <- current_q</pre>
 ptraj[1,] <- p
```

Then the action comes in a loop over leapfrog steps. L steps are taken, using the gradient to compute a linear approximation of the log-posterior surface at each point.

```
# Alternate full steps for position and momentum
for ( i in 1:L ) {
 q = q + epsilon * p # Full step for the position
  # Make a full step for the momentum, except at end of trajectory
 if ( i!=L ) {
      p = p - epsilon * grad_U(q)
      ptraj[i+1,] <- p
```



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Calculus is a superpower

Hamiltonian Monte Carlo needs gradients How does it get them? Write them yourself or... Auto-diff: Automatic differentiation Symbolic derivatives of your model code Used in many machine learning approaches; "Backpropagation" is special case

	-	2
∂B_x	∂B_y	<u>ə</u> 1
∂x	∂x	∂
∂B_x	∂B_{y}	∂I
дy	дy	∂_{i}
∂B_x	∂B_{y}	∂I
∂z	∂z	∂

J =





Stan

About Stan

Stan is a state-of-the-art platform for statistical modeling and high-performance statistical computation. Thousands of users rely on Stan for statistical modeling, data analysis, and prediction in the social, biological, and physical sciences, engineering, and business.





Stanisław Ulam and his daughter Claire with MANIAC

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-

6 6





Example: Divorce data

```
library(rethinking)
data(WaffleDivorce)
d <- WaffleDivorce
dat <- list(</pre>
    D = standardize(d$Divorce),
    M = standardize(d$Marriage),
    A = standardize(d$MedianAgeMarriage)
f <- alist(
         D ~ dnorm(mu,sigma),
         mu < -a + bM \star M + bA \star A,
         a \sim dnorm(0, 0.2),
         bM \sim dnorm(0, 0.5),
         bA \sim dnorm(0, 0.5),
         sigma ~ dexp(1)
mq <- quap( f , data=dat )</pre>
```

 $D_{i} \sim \text{Normal}(\mu_{i}, \sigma)$ $\mu_{i} = \alpha + \beta_{M}M_{i} + \beta_{A}A_{i}$ $\alpha \sim \text{Normal}(0, 0.2)$ $\beta_{M} \sim \text{Normal}(0, 0.5)$ $\beta_{A} \sim \text{Normal}(0, 0.5)$ $\sigma \sim \text{Exponential}(1)$

Example: Divorce data

f <- alist(D ~ dnorm(mu,sigma), mu < -a + bM + bA + a $a \sim dnorm(0, 0.2),$ $bM \sim dnorm(0, 0.5),$ $bA \sim dnorm(0, 0.5),$ sigma ~ dexp(1)mq <- quap(f , data=dat)</pre> library(cmdstanr) mHMC <- ulam(f , data=dat)</pre>

 $D_{i} \sim \text{Normal}(\mu_{i}, \sigma)$ $\mu_{i} = \alpha + \beta_{M}M_{i} + \beta_{A}A_{i}$ $\alpha \sim \text{Normal}(0, 0.2)$ $\beta_{M} \sim \text{Normal}(0, 0.5)$ $\beta_{A} \sim \text{Normal}(0, 0.5)$ $\sigma \sim \text{Exponential}(1)$

Example: Divorce data

f <	- alis	st(
		o ~ dn	orm(m	nu,sigr	na),		
	ľ	nu <-	a + b	• M * M	bA*A,		
	> pred	cis(mHN	1C)				
		mean	sd	5.5%	94.5%	n_eff	Rhat4
	а	0.00	0.10	-0.16	0.16	1632	1
	ЬM	-0.06	0.17	-0.32	0.21	1137	1
	bA	-0.61	0.17	-0.86	-0.34	1160	1
	sigma	0.83	0.09	0.70	0.99	1504	1
mq	>						
lib	rary(mdsta	nr)				

mHMC <- ulam(f , data=dat)

 $D_{i} \sim \text{Normal}(\mu_{i}, \sigma)$ $\mu_{i} = \alpha + \beta_{M}M_{i} + \beta_{A}A_{i}$ $\alpha \sim \text{Normal}(0, 0.2)$ $\beta_{M} \sim \text{Normal}(0, 0.5)$ $\beta_{A} \sim \text{Normal}(0, 0.5)$ $\sigma \sim \text{Exponential}(1)$

Pure Stan approach

ulam() just builds Stan code

Stan code is portable, runs on anything

Learn Stan, work in any scripting language

```
// stancode(mHMC)
data{
    // the observed variables
    vector[50] D;
    vector[50] A;
    vector[50] M;
}
parameters{
    // the unobserved variables
    real a;
    real bM;
    real bA;
    real<lower=0> sigma;
model{
    // compute the log posterior probability
    vector[50] mu;
    sigma ~ exponential( 1 );
    bA \sim normal(0, 0.5);
    bM \sim normal(0, 0.5);
    a ~ normal( 0 , 0.2 );
    for ( i in 1:50 ) {
        mu[i] = a + bM * M[i] + bA * A[i];
    D ~ normal( mu , sigma );
```

```
// stancode(mHMC)
data{
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    vector[50] D;
    vector[50] A;
    vector[50] M;
parameterst
    // the unobserved variables
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    vector[50] mu;
    sigma ~ exponential( 1 );
    bA \sim normal(0, 0.5);
    bM \sim normal(0, 0.5);
    a ~ normal( 0 , 0.2 );
    for ( i in 1:50 ) {
        mu[i] = a + bM * M[i] + bA * A[i];
    D ~ normal( mu , sigma );
```

Must declare the type of each observed variable so Stan can catch errors and know what operations are allowed



```
// stancode(mHMC)
data{
    // the observed variables
    vector[50] D;
    vector[50] A;
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    bA \sim normal(0, 0.5);
    bM \sim normal(0, 0.5);
    a ~ normal( 0 , 0.2 );
    for ( i in 1:50 ) {
        mu[i] = a + bM * M[i] + bA * A[i];
    D ~ normal( mu , sigma );
```

Must declare the type of each observed variable so Stan can catch errors and know what operations are allowed

Unobserved variables also need checks and constraints. Declared here.



```
// stancode(mHMC)
data{
    // the observed variables
    vector[50] D;
    vector[50] A;
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    real a;
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    real bA;
    real<lower=0> sigma;
model{
    // compute the log posterior probability
    vector[50] mu;
    sigma ~ exponential( 1 );
    bA \sim normal(0, 0.5);
    bM ~ normal( 0 , 0.5 );
    a ~ normal( 0 , 0.2 );
    for ( i in 1:50 ) {
        mu[i] = a + bM * M[i] + bA * A[i];
    D ~ normal( mu , sigma );
```

Must declare the type of each observed variable so Stan can catch errors and know what operations are allowed

Unobserved variables also need checks and constraints. Declared here.

Declare the distributional parts of the model, sufficient to compute posterior probability

In big models, this part can be very complex



Pure Stan approach

Save Stan code as own file

mHMC_stan <- cstan(file="08_mHMC.stan"
, data=dat)</pre>

Extract samples and proceed as usual

post <- extract.samples(mHMC_stan)</pre>

```
// stancode(mHMC)
data{
    // the observed variables
    vector[50] D;
    vector[50] A;
    vector[50] M;
parameters{
    // the unobserved variables
    real a;
    real bM;
    real bA;
    real<lower=0> sigma;
model{
    // compute the log posterior probability
    vector[50] mu;
    sigma ~ exponential( 1 );
    bA \sim normal(0, 0.5);
    bM \sim normal(0, 0.5);
    a ~ normal( 0 , 0.2 );
    for ( i in 1:50 ) {
        mu[i] = a + bM * M[i] + bA * A[i];
    D ~ normal( mu , sigma );
```

Drawing the Markov Owl

- Complex machinery, but lots of diagnostics
- (1) Trace plots
- (2) Trace rank plots
- (3) R-hat convergence measure
- (4) Number of effective samples
- (5) Divergent transitions











Need more than 1 chain to check convergence

Convergence: Each chain explores the right distribution and every chain explores the same distribution

library(cmdstanr) mHMC <- ulam(f , data=dat)</pre> mHMC <- ulam(f , data=dat , chains=4 , cores=4)</pre>



 $D_i \sim \text{Normal}(\mu_i, \sigma)$ $\mu_i = \alpha + \beta_M M_i + \beta_A A_i$ $\alpha \sim \text{Normal}(0,0.2)$ $\beta_M \sim \text{Normal}(0,0.5)$ $\beta_A \sim \text{Normal}(0,0.5)$ $\sigma \sim \text{Exponential}(1)$









Trace rank (Trank) plots



Trace rank (Trank) plots









R-hat

When chains converge:

(1) Start and end of each chain explores same region

(2) Independent chains explore same region

R-hat is a ratio of variances: As total variance shrinks to average variance within chains, R-hat approaches 1

NO GUARANTEES; NOT A TEST

> pre	<pre>> precis(mHMC)</pre>					
	mean	sd	5.5%	94.5%	n_eff	R
а	0.00	0.10	-0.16	0.16	1632	
ЬM	-0.06	0.17	-0.32	0.21	1137	
bA	-0.61	0.17	-0.86	-0.34	1160	
sigma	0.83	0.09	0.70	0.99	1504	
>						







Estimate of number of effective samples

"How long would the chain be, if each sample was independent of the one before it?"

When samples are autocorrelated, you have fewer *effective* samples

> precis(mHMC)						
	mean	sd	5.5%	94.5%	n_eff	R
а	0.00	0.10	-0.16	0.16	1632	
ЬM	-0.06	0.17	-0.32	0.21	1137	
bA	-0.61	0.17	-0.86	-0.34	1160	
sigma	0.83	0.09	0.70	0.99	1504	
>						









Divergent transitions

Divergent transition: A kind of rejected proposal

Simulation *diverges* from true path

Many DTs: poor exploration & possible bias

Will discuss again in later lecture









pred	cis(m9.2	2)				
	mean	sd	5.5%	94.5%	n_eff	Rha
lpha	-27.98	280.33	-485.11	291.74	121	1
igma	390.82	993.07	1.83	1870.86	169	1
es=3)					





Warning: 108 of 1500 (7.0%) transitions ended with a divergence. This may indicate insufficient exploration of the posterior distribution. Possible remedies include: * Increasing adapt_delta closer to 1 (default is 0.8) * Reparameterizing the model (e.g. using a non-centered parameterization) * Using informative or weakly informative prior distributions

pred	cis(m9.2	2)				
	mean	sd	5.5%	94.5%	n_eff	Rha
lpha	-27.98	280.33	-485.11	291.74	121	1
igma	390.82	993.07	1.83	1870.86	169	1
es=3)					









The Folk Theorem of Statistical Computing

"When you have computational problems, often there's a problem with your model."

Andrew Gelman Spider-Man of Bayesian data analysis



```
y <- c(-1,1)
set.seed(11)
m9.2 <- ulam(
    alist(
        y ~ dnorm( mu , sigma ),
        mu <- alpha,
        alpha ~ dnorm( 0 , 1000 ),
        sigma ~ dexp( 0.0001 )
        ) , data=list(y=y) , chains=3 ,
cores=3 )</pre>
```

> pred	cis(m9.2	2)				
	mean	sd	5.5%	94.5%	n_eff	Rhat4
alpha	-27.98	280.33	-485.11	291.74	121	1.01
sigma	390.82	993.07	1.83	1870.86	169	1.03
>						

<pre>> precis(m9.3)</pre>						
	mean	sd	5.5%	94.5%	n_eff	Rhat4
alpha	0.06	1.07	-1.62	1.80	424	1.01
sigma	1.51	0.80	0.65	3.02	501	1.00
>						







El Pueblo Unido

Desktop MCMC has been a revolution in scientific computing

Custom scientific modeling

High-dimension

Propagate measurement error

Do not "pipette by mouth"





Sir David Spiegelhalter

Course Schedule

Week 1	Bayesian inference	Chapters 1, 2, 3
Week 2	Linear models & Causal Inference	Chapter 4
Week 3	Causes, Confounds & Colliders	Chapters 5 & 6
Week 4	Overfitting / MCMC	Chapters 7, 8, 9
Week 5	Generalized Linear Models	Chapters 10, 11
Week 6	Integers & Other Monsters	Chapters 11 & 12
Week 7	Multilevel models I	Chapter 13
Week 8	Multilevel models II	Chapter 14
Week 9	Measurement & Missingness	Chapter 15
Week 10	Generalized Linear Madness	Chapter 16

https://github.com/rmcelreath/stat_rethinking_2022

