## Statistical Rethinking



## 08: Markov chain Monte Carlo





## 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)




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

(2) Find population of proposal 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.
(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.

(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.
(4) Move to proposal, with probability $=\frac{p_{5}}{p_{4}}$


1


2


3

(5) Repeat from (1)
(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.
(4) Move to proposal, with probability $=\frac{p_{5}}{p_{4}}$
(5) Repeat from (1)


1



2





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
"Markov chain Monte Carlo"


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

Easy to write, very general, often inefficient

## 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

AND
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.

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

## Equation of state calculations by fast computing machines

 ..., AW Rosenbluth, MN Rosenbluth... - The journal of ..., 1953-aip.scitation.orgA 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.

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.




## 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

## 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

## High probability

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 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 log posterior, as stated before in the main text:

$$
\sum \log p\left(y_{i} \mid \mu_{y}, 1\right)+\sum \log p\left(x_{i} \mid \mu_{x}, 1\right)+\log p\left(\mu_{y} \mid 0,0.5\right)+\log p\left(\mu_{x}, 0,0.5\right)
$$

So its just four calls to dnorm really
R code
9.5 $\# U$ needs to return neg-log-probability

```
u <- function( a, a=0, b=1,k=0,d=1)
    muy<- q[1]
    U <- sum(dnorm(y,muy, 1, log=TRUE)) + sum(dnorm(x,mux, 1, log=TRUE)) +
        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:

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

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

$$
\frac{\partial U}{\partial \mu_{x}}=\frac{\partial \log \mathrm{N}\left(x \mid \mu_{x}, 1\right)}{\partial \mu_{x}}+\frac{\partial \log \mathrm{N}\left(\mu_{x} \mid 0,0.5\right)}{\partial \mu_{x}}=\sum_{i} \frac{x_{i}-\mu_{x}}{1^{2}}+\frac{0-\mu_{x}}{0.5^{2}}
$$

And the gradient for $\mu_{y}$ has the same form. Now in code form:
\# need vector of partial derivatives of $U$ with respect to vector
U_gradient <-il
muy $<-\mathrm{q}[1]$
mux $<-\mathrm{g}[2]$
$G 1<-\operatorname{sum}(y-$ muy $)+(a-$ muy $) / b^{\wedge} 2 \# d U / d$ muy
$G 2<-\operatorname{sum}(x-\operatorname{mux})+(k-$ mux $) / d^{\wedge} 2 \# d d / d m u x$
return( c( -G1, -G2) ) \# negative bc energy is neg-log-prob
\# test data
set. seed (7)
<-rnorm(50)
$x<-r n o r m(50)$
$x<-$ as.numeric(scale $(x)$
$x<-$ as.numeric $(s c a t e()$
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 defini ion. Now we are ready to visit the heart. To understand some of the details here, you should read adoren form

```
ibrary(shape) # for fancy arrows
Q <- list()
Q$q <- c(-0.1,0.2)
pr <- 0.3
lol}\begin{array}{l}{\mathrm{ pr <- 0.3 ( Nlot( NULL, ylab="muy", xlab="mux", xlim=c(-pr,pr),ylim=c(-pr,pr))}}\\{\mathrm{ step <- 0.03 }}
step <- 0.03 
n_samples <- 4
path_col <- col.alpha("black",0.5)
points( Q$q[1], Q$q[2], pch=4, col="black" )
for(i in 1:n_samples )
    Q <- HMC2(U, U_gradient, step, Usa
        Q <- HMC2(U, U_gradient, step, L, Q$q
        for ( }\textrm{j}\mathrm{ in 1:L) {
            K0 <- sum(Q$ptraj[j,]^2)/2 # kinetic energy
            lines( Q$straj[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]
            Mows( Q$traj[L,1],Q$traj[L,2],Q$
            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"))
```

3

The function HMC2 is built into rethinking. It is based upon one of Radford Neal's example scripts. ${ }^{15}$ It isn't actually too complicated. Let's tour through it, one step at a time, to take the magic away. This 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.
    # Make a half step for momentum at the beginning
    p=p-epsilon * grad_U(q)/2
    p initialize mookradu(q) /2
    gtraj <- matrix(NA , row=L+1, ncol=l trajectory
    qtraj <- matrix(NA, nrow=L+1,ncol=length(q)
    ptraj <- qtra
    qtraj[1,]<-current_q
    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 + epsilon * p # Full step for the position
    # Make a full step for the momentum, except at end of trajectory
        p=p - epsilon * grad_U(q)
            ptraj[i+1,] <- p
}
```


## 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

mc-stan.org
Stanisław Ulam (1909-1984)

## 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.




## Example: Divorce data

```
library(rethinking)
data(WaffleDivorce)
d <- WaffleDivorce
dat <- list(
    D = standardize(d$Divorce),
    M = standardize(d$Marriage),
    A = standardize(d$MedianAgeMarriage)
)
f<- alist(
    D ~ dnorm(mu,sigma),
    mu <- a + bM*M + bA*A,
    a ~ dnorm(0,0.2),
    bM ~ dnorm(0,0.5),
    bA ~ dnorm(0,0.5),
    sigma ~ dexp(1)
    )
mq <- quap( f , data=dat )
\[
\begin{aligned}
D_{i} & \sim \operatorname{Normal}\left(\mu_{i}, \sigma\right) \\
\mu_{i} & =\alpha+\beta_{M} M_{i}+\beta_{A} A_{i} \\
\alpha & \sim \operatorname{Normal}(0,0.2) \\
\beta_{M} & \sim \operatorname{Normal}(0,0.5) \\
\beta_{A} & \sim \operatorname{Normal}(0,0.5) \\
\sigma & \sim \operatorname{Exponential}(1)
\end{aligned}
\]

\section*{Example: Divorce data}
```

f <- alist(
D ~ dnorm(mu, sigma),
mu <- a + bM*M + bA*A,
a ~ dnorm(0,0.2),
bM ~ dnorm(0,0.5),
bA ~ dnorm(0,0.5),
sigma ~ dexp(1)
)

```
\(\mathrm{mq}<-\) quap ( f , data=dat )
library (cmdstanr)
\[
\begin{aligned}
D_{i} & \sim \operatorname{Normal}\left(\mu_{i}, \sigma\right) \\
\mu_{i} & =\alpha+\beta_{M} M_{i}+\beta_{A} A_{i} \\
\alpha & \sim \operatorname{Normal}(0,0.2) \\
\beta_{M} & \sim \operatorname{Normal}(0,0.5) \\
\beta_{A} & \sim \operatorname{Normal}(0,0.5) \\
\sigma & \sim \operatorname{Exponential}(1)
\end{aligned}
\]
```

mHMC <- ulam( f , data=dat )

```

\section*{Example: Divorce data}
```

f <- alist(
D ~ dnorm(mu,sigma),
mu <- a + bM*M + bA*A,
> precis(mHMC)
mean sd 5.5% 94.5% n_eff Rhat4
a 0.00 0.10 -0.16 0.16 1632 1
bM -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
mq
*

```
\(D_{i} \sim \operatorname{Normal}\left(\mu_{i}, \sigma\right)\)
\(\mu_{i}=\alpha+\beta_{M} M_{i}+\beta_{A} A_{i}\)
\(\alpha \sim \operatorname{Normal}(0,0.2)\)
\(\beta_{M} \sim \operatorname{Normal}(0,0.5)\)
\(\beta_{A} \sim \operatorname{Normal}(0,0.5)\)
\(\sigma \sim\) Exponential(1)
library (cmdstanr)
mHMC <- ulam( f , data=dat )

\section*{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 ~ 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 );

```
\}
```

// stancode(mHMC)
data{
// the observed variables
vector[50] D;
vector[50] A;
vector[50] M;
}
par amelers{
// 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 ~ 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 );

```
\}
```

// 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 ~ 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 );
}

```
```

// 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 ~ 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

\section*{Pure Stan approach}

\section*{Save Stan code as own file}
```

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

```
```

post <- extract.samples(mHMC_stan)

```
```

// 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 ~ 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 );
}

```

\section*{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

\section*{Trace plots}


\section*{Trace plots}


Need more than 1 chain to check convergence

Convergence: Each chain explores the \(D_{i} \sim \operatorname{Normal}\left(\mu_{i}, \sigma\right)\) right distribution and every chain \(\mu_{i}=\alpha+\beta_{M} M_{i}+\beta_{A} A_{i}\) \(\alpha \sim \operatorname{Normal}(0,0.2)\) explores the same distribution
\(\beta_{M} \sim \operatorname{Normal}(0,0.5)\)
\(\beta_{A} \sim \operatorname{Normal}(0,0.5)\)
\(\sigma \sim \operatorname{Exponential(1)}\)
```

mHMC <- ulam( f , data=dat , chains=4 , cores=4 )

```

\section*{Trace plots}


\section*{Trace plots}





\section*{Trace plots}





\section*{Trace plots}





\section*{Trace rank (Trank) plots}


\section*{Trace rank (Trank) plots}


\section*{R-hat}

When chains converge:
(1) Start and end of each chain explores
\begin{tabular}{lrrrrrrr}
\hline \multicolumn{8}{l|}{ precis(mHMC) } \\
& mean & sd & \(5.5 \%\) & \(94.5 \%\) & n_eff & Rhat4 \\
a & 0.00 & 0.10 & -0.16 & 0.16 & 1632 & 1 \\
bM & -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 \\
\(>\) & & & & & & \\
\hline
\end{tabular} 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

\section*{NO GUARANTEES; NOT A TEST}
n_eff

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



\section*{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


\section*{Bad chains}
```

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 )

```

\section*{Bad chains}
```

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 )

\section*{Bad chains}
```

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 )

```
```

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

```


\section*{The Folk Theorem of Statistical Computing}
"When you have computational problems, often there's a problem with your model."

\section*{Andrew Gelman}

Spider-Man of Bayesian data analysis

\section*{Bad chains}
```

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 )

```
```

m9.3 <- ulam(
alist(
y ~ dnorm( mu , sigma ),
mu <- alpha,
alpha ~ dnorm( 1 , 10 ),
sigma ~ dexp( 1 )
) , data=list(y=y) , chains=3 , cores=3 )

```

\section*{> precis(m9.2)}
mean sd 5.5\% 94.5\% n_eff Rhat4
alpha \(-27.98280 .33-485.11 \quad 291.74 \quad 121 \quad 1.01\)
sigma \(390.82993 .07 \quad 1.831870 .86 \quad 169 \quad 1.03\)

\section*{> precis(m9.3) \\ mean sd 5.5\% 94.5\% n_eff Rhat4 \\ alpha \(0.06 \quad 1.07-1.62 \quad 1.80 \quad 424 \quad 1.01\) \\ \(\begin{array}{lllllll}\text { sigma } & 1.51 & 0.80 & 0.65 & 3.02 & 501 & 1.00\end{array}\)}


\section*{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

\section*{Course Schedule}
\begin{tabular}{|l|l|l|}
\hline Week 1 & Bayesian inference & Chapters 1, 2, 3 \\
\hline Week 2 & Linear models \& Causal Inference & Chapter 4 \\
\hline Week 3 & Causes, Confounds \& Colliders & Chapters 5 \& 6 \\
\hline Week 4 & Overfitting / MCMC & Chapters 7, 8, 9 \\
\hline Week 5 & Generalized Linear Models & Chapters 10, 11 \\
\hline Week 6 & Integers \& Other Monsters & Chapters 11 \& 12 \\
\hline Week 7 & Multilevel models I & Chapter 13 \\
\hline Week 8 & Multilevel models II & Chapter 14 \\
\hline Week 9 & Measurement \& Missingness & Chapter 15 \\
\hline Week 10 & Generalized Linear Madness & Chapter 16 \\
\hline
\end{tabular}
https://github.com/rmcelreath/stat_rethinking_2022```

