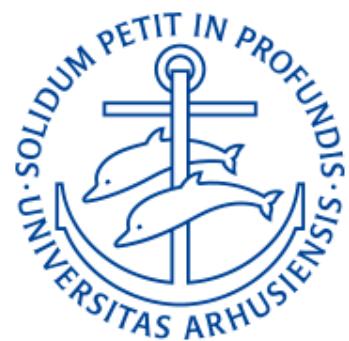


Methods 4 - 8

Chris Mathys



BSc Programme in Cognitive Science

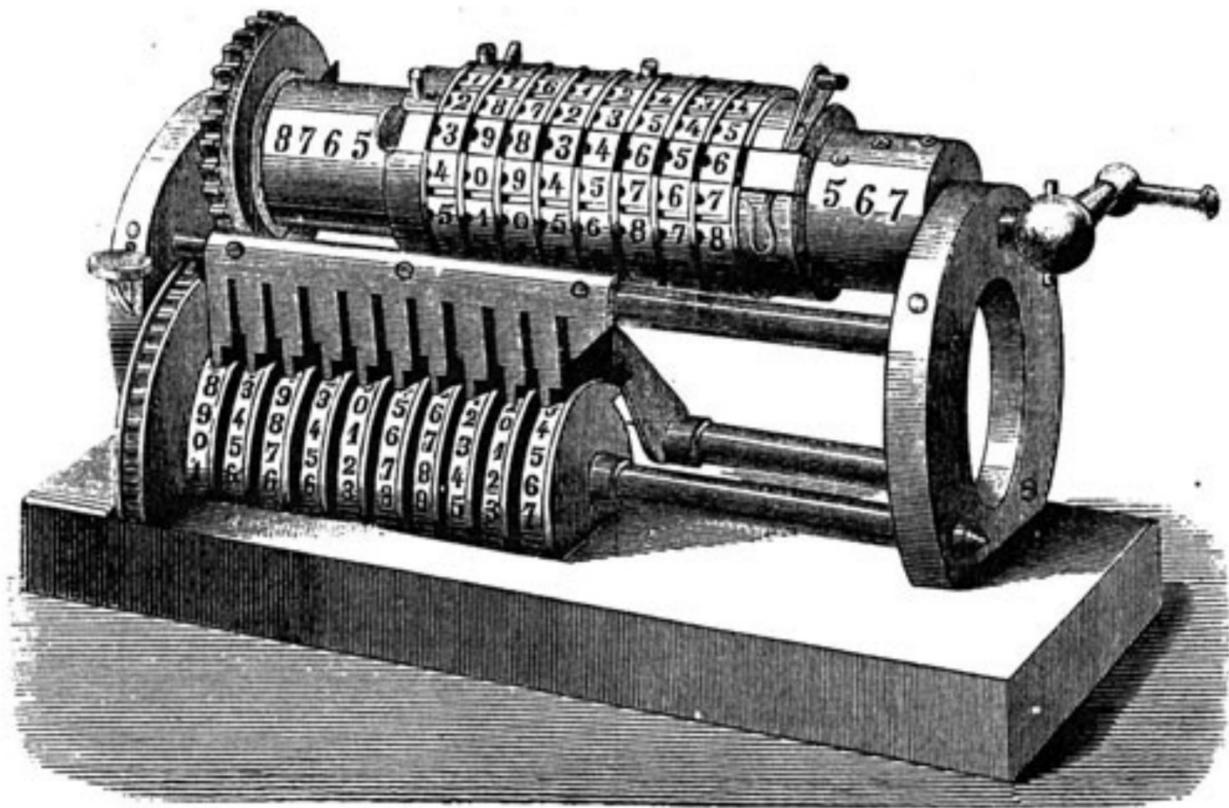
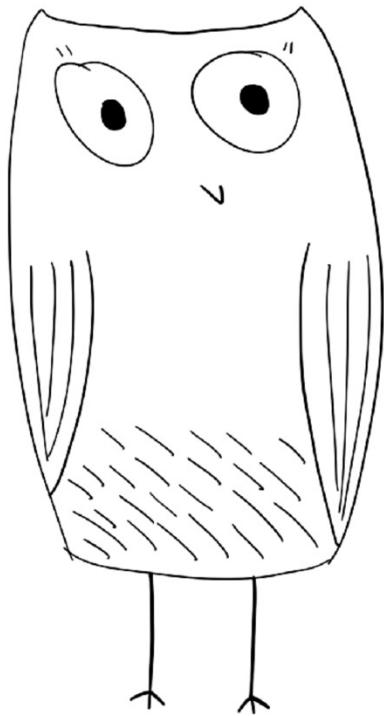
Spring 2023

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

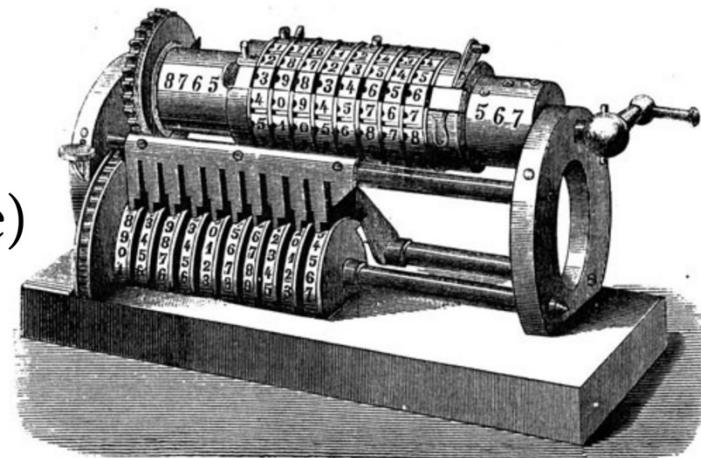


aNA1YzE rEA1 DatA



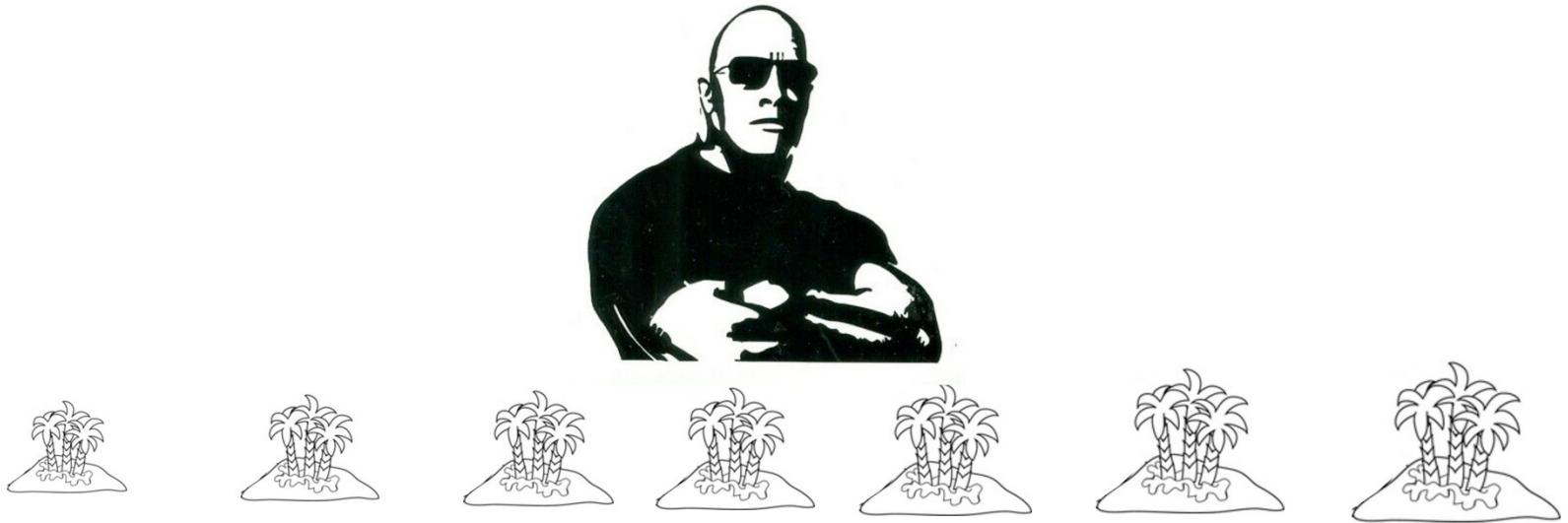
Computing the posterior

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





King Markov

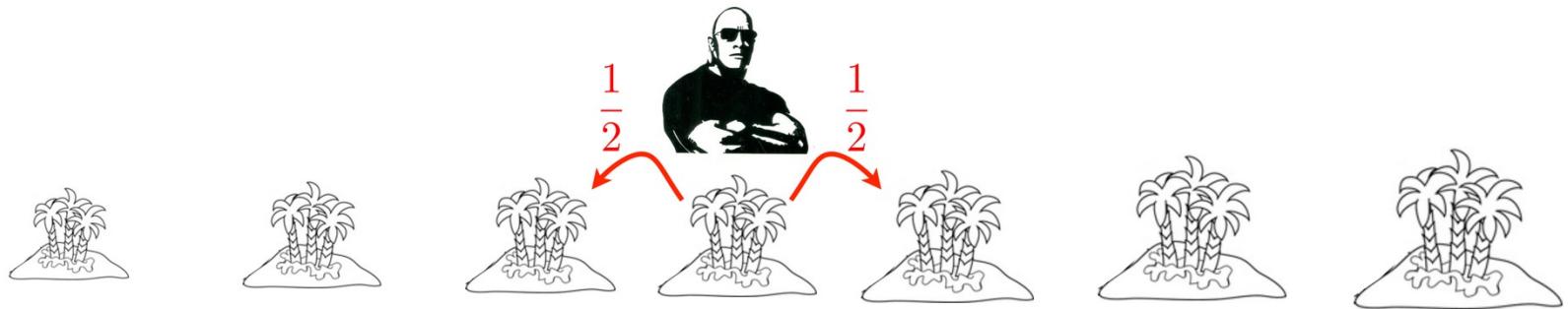


The Metropolis Archipelago

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

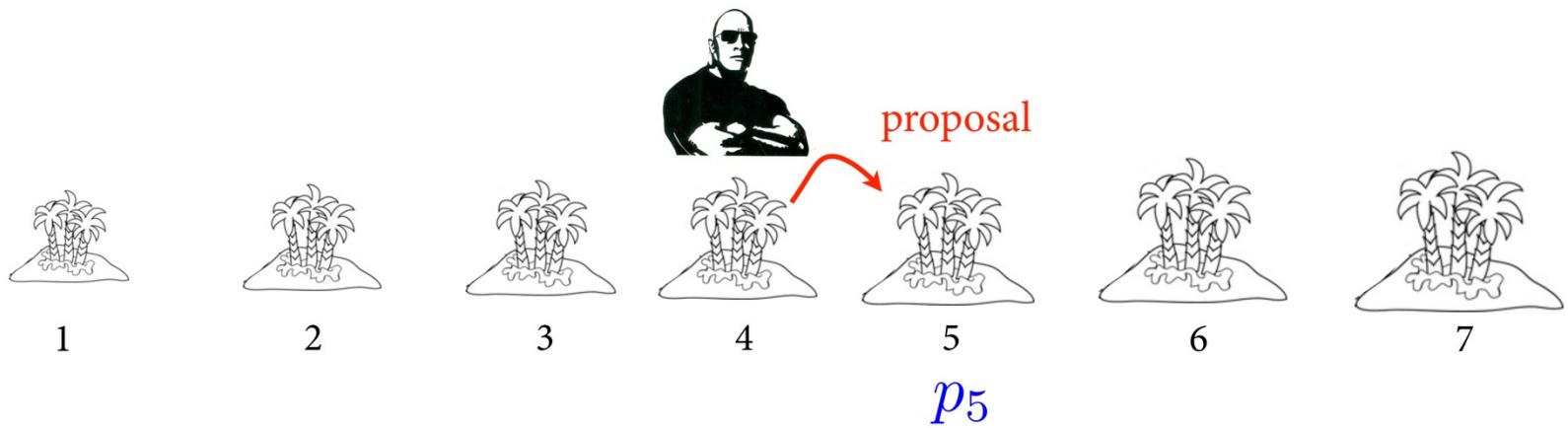


Here's how he does it...



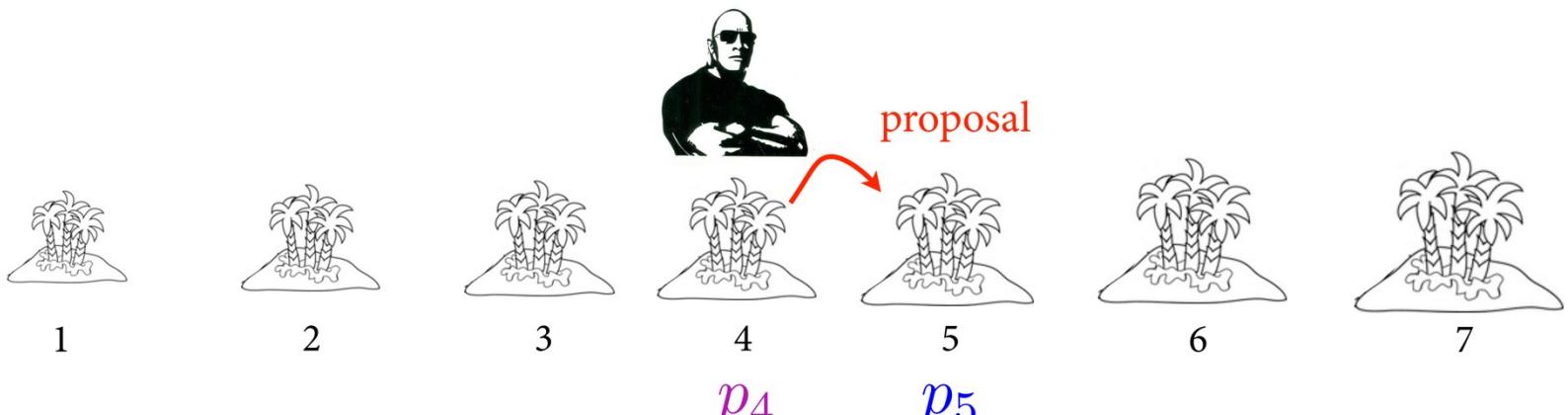
(1) Flip a coin to choose island on left or right.
Call it the “proposal” island.

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Call it the “proposal” island.



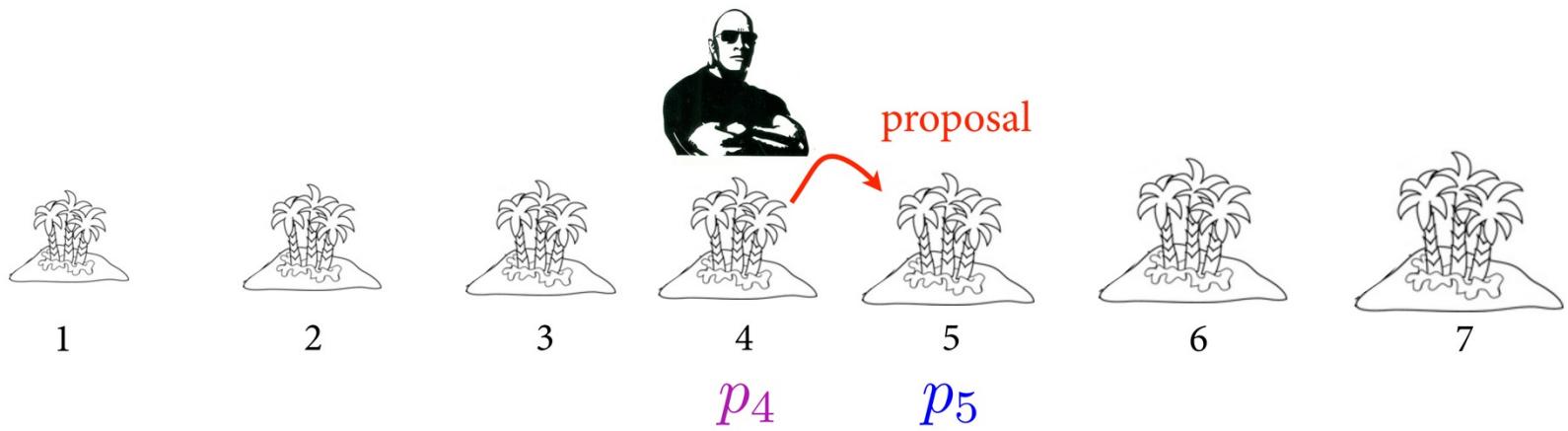
(2) Find population of proposal island.

- (1) Flip a coin to choose island on left or right.
Call it the “proposal” island.
- (2) Find population of proposal island.



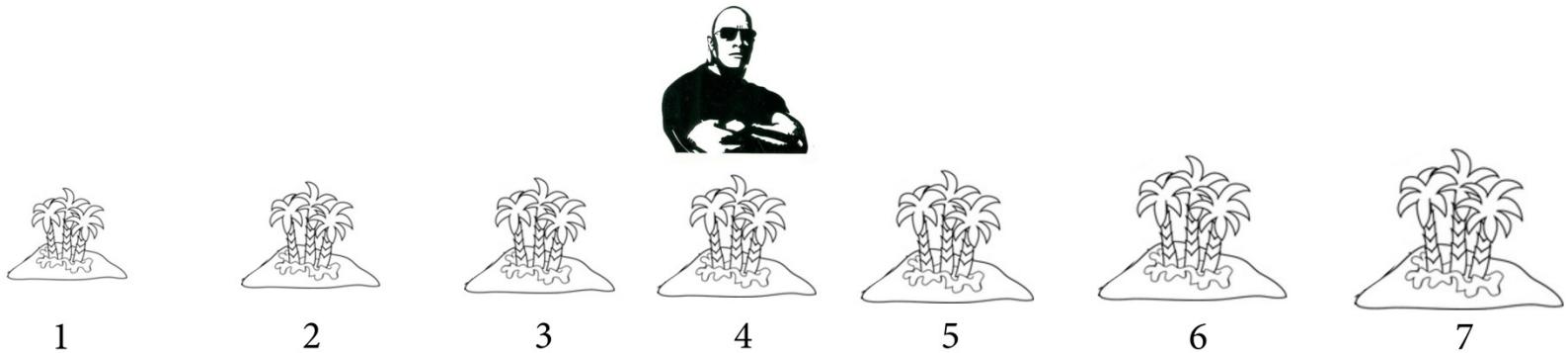
- (3) Find population of current island.

- (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 = $\frac{p_5}{p_4}$



(5) Repeat from (1)

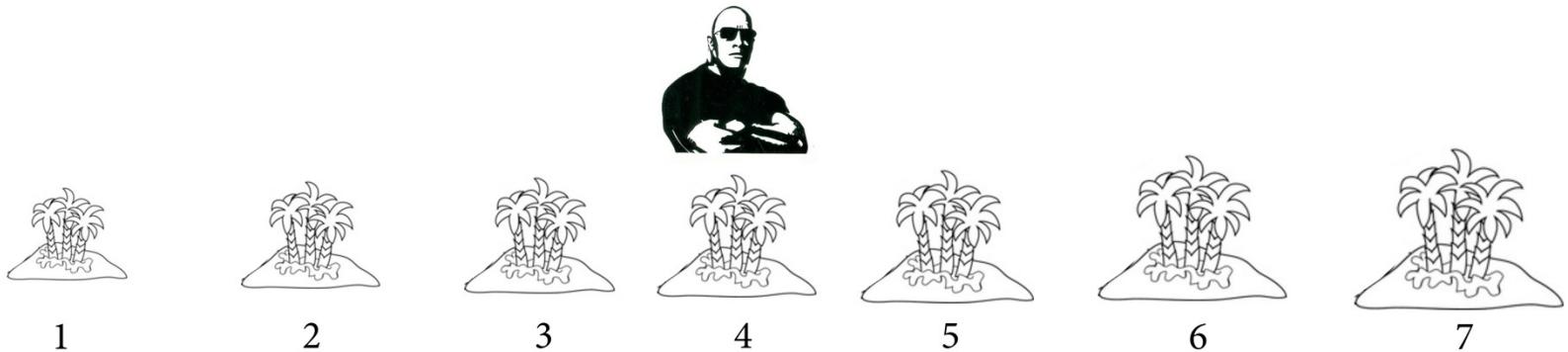
(1) Flip a coin to choose island on left or right.
Call it the “proposal” island.

(2) Find population of proposal island.

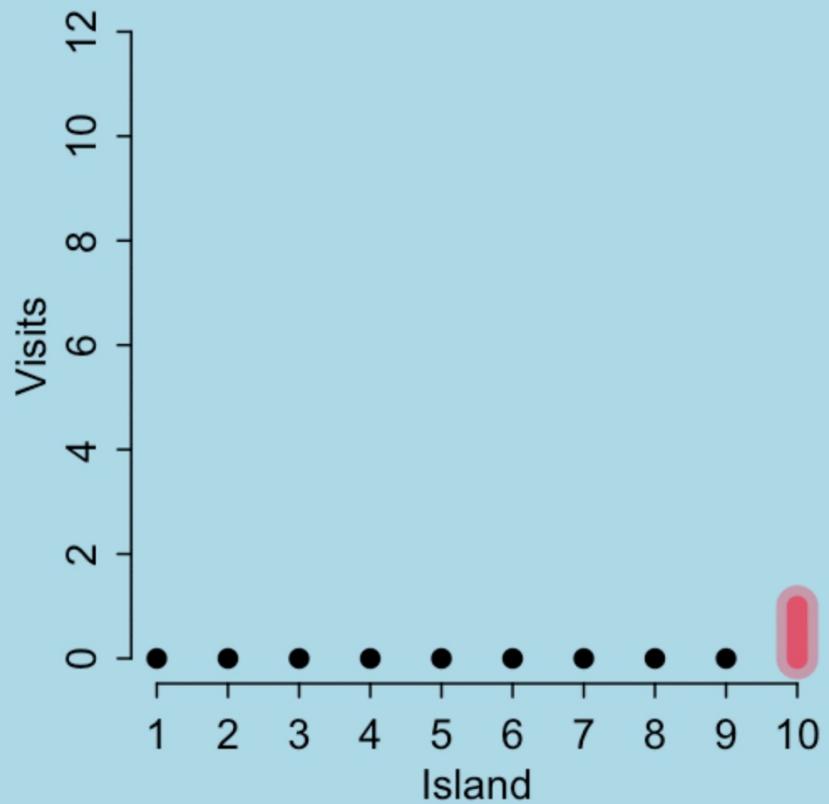
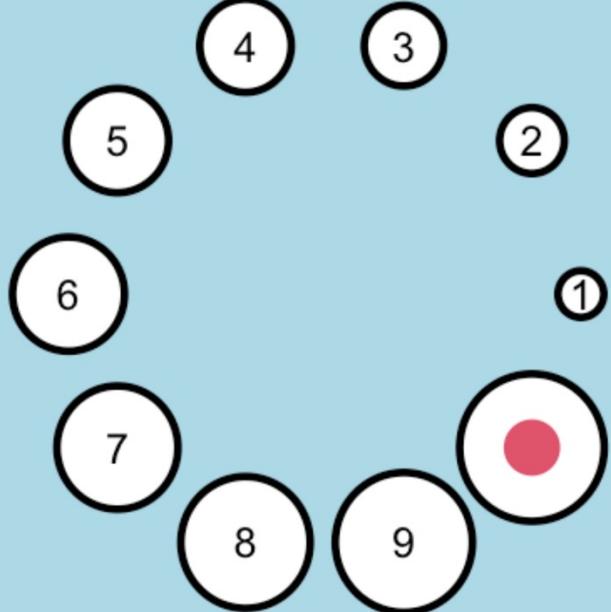
(3) Find population of current island.

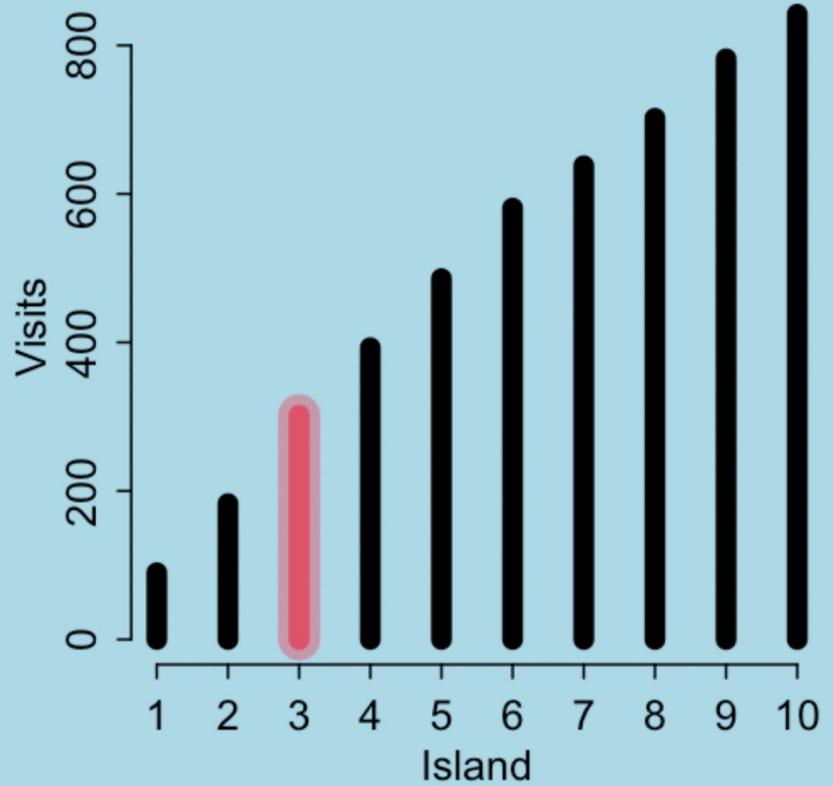
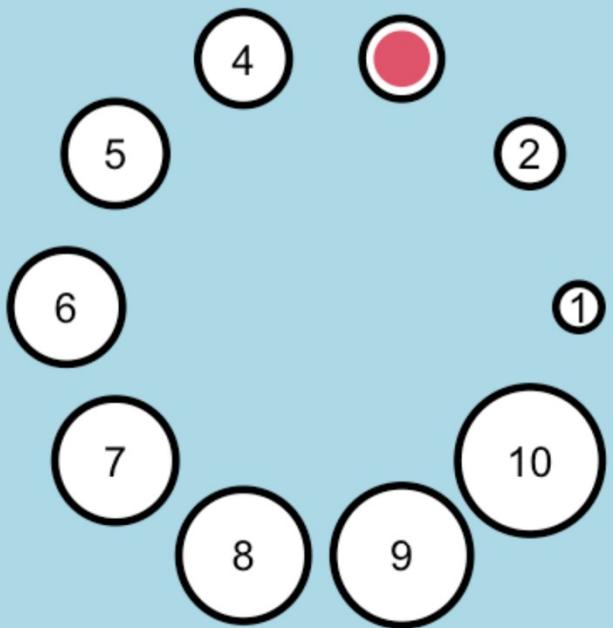
(4) Move to proposal, with probability = $\frac{p_5}{p_4}$

(5) Repeat from (1)



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

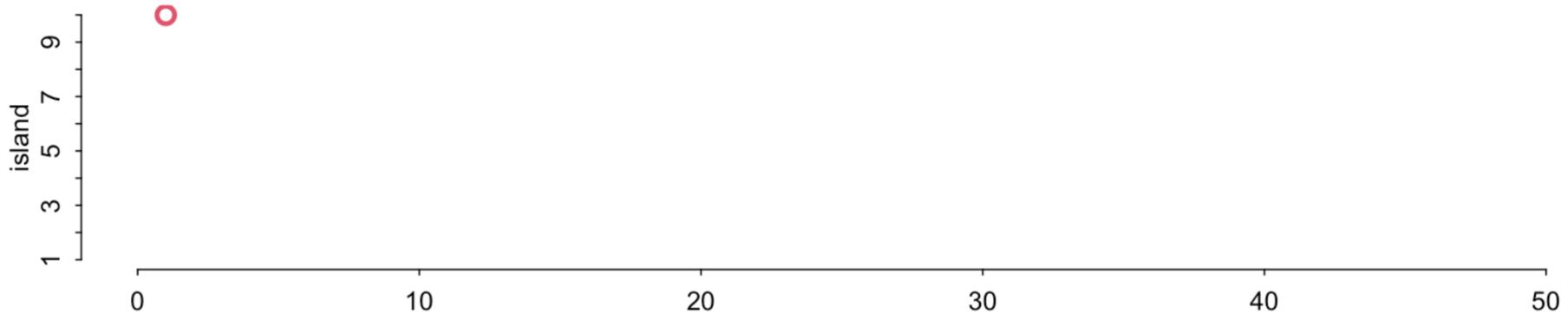
“Population size”: posterior probability

Visit each parameter value in proportion to its posterior probability

Any number of dimensions (parameters)



“Markov chain Monte Carlo”

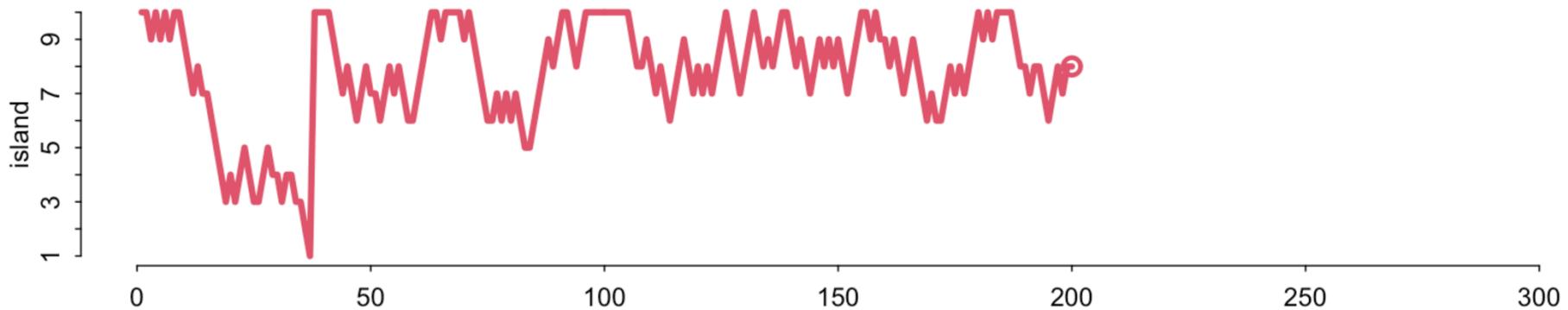


Chain: Sequence of draws from distribution

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.org

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[Save](#) [Cite](#) Cited by 47206 Related articles All 29 versions

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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

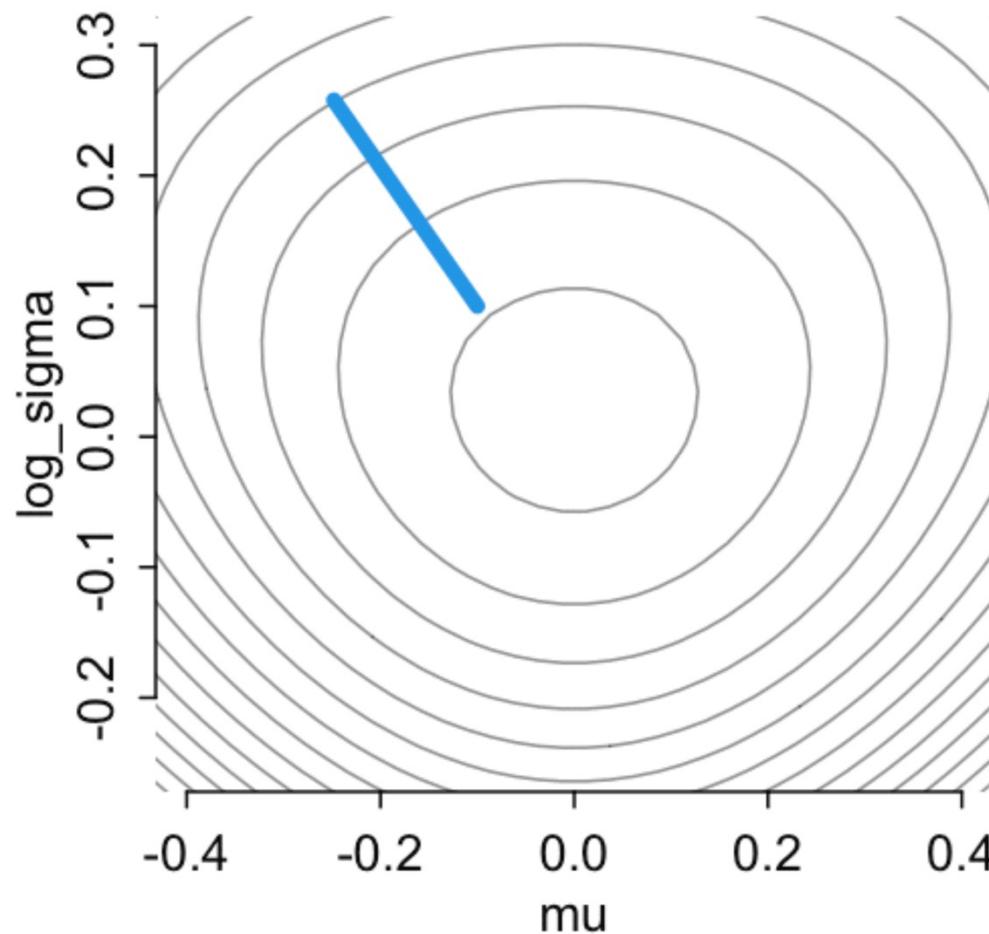
Handbook of Markov Chain Monte Carlo

Edited by

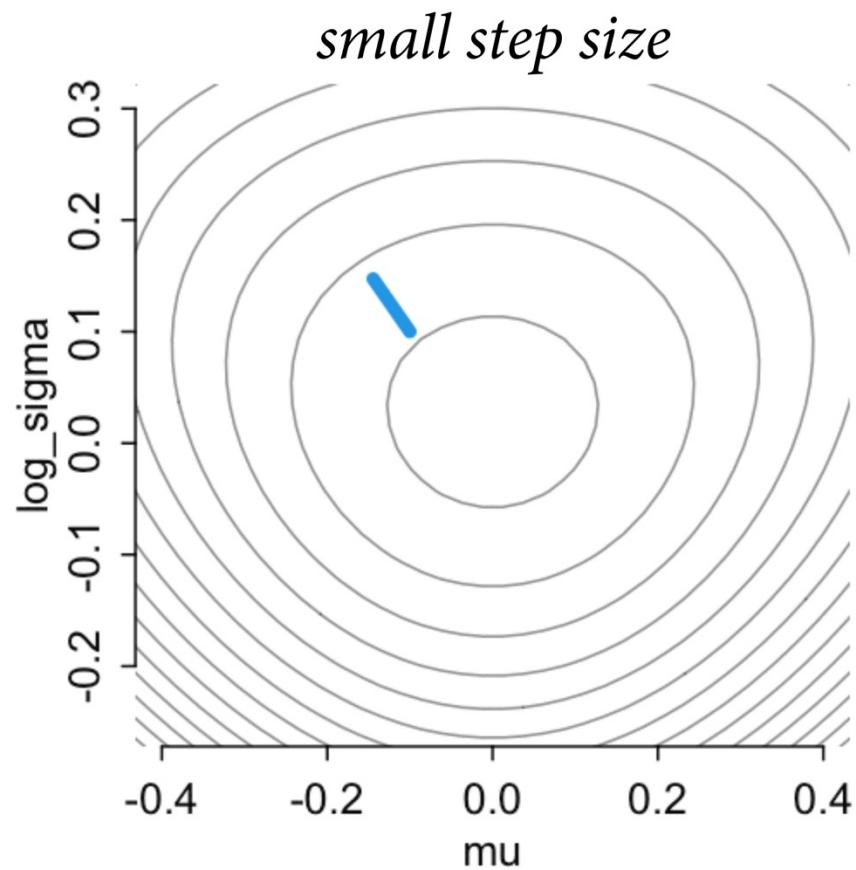
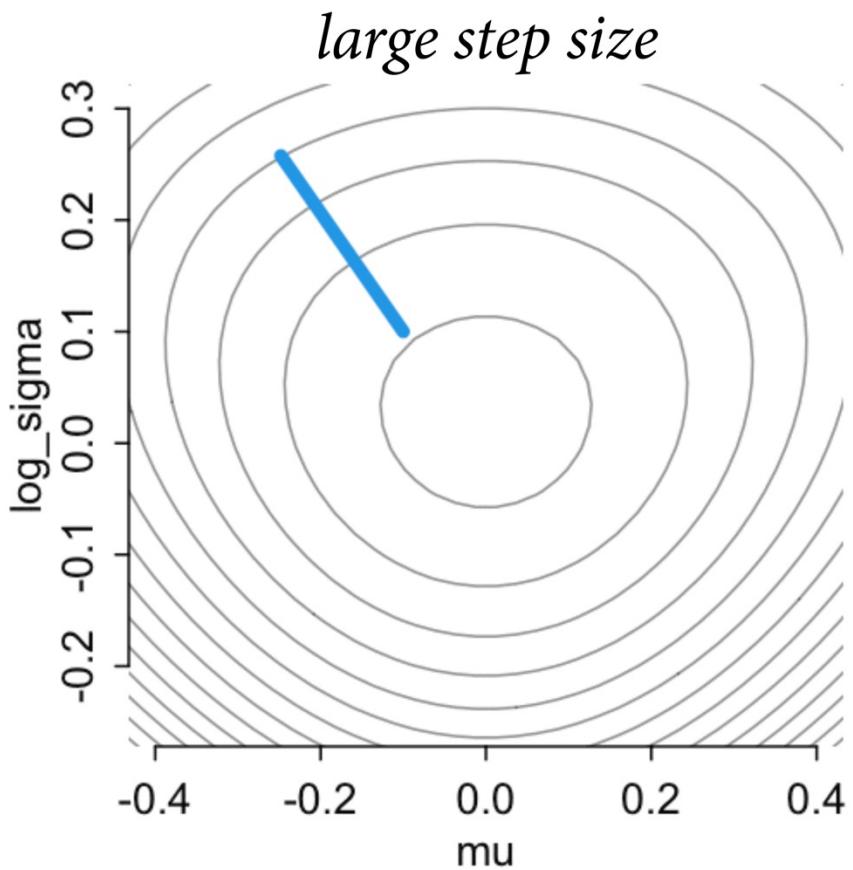
Steve Brooks
Andrew Gelman
Galin L. Jones
Xiao-Li Meng



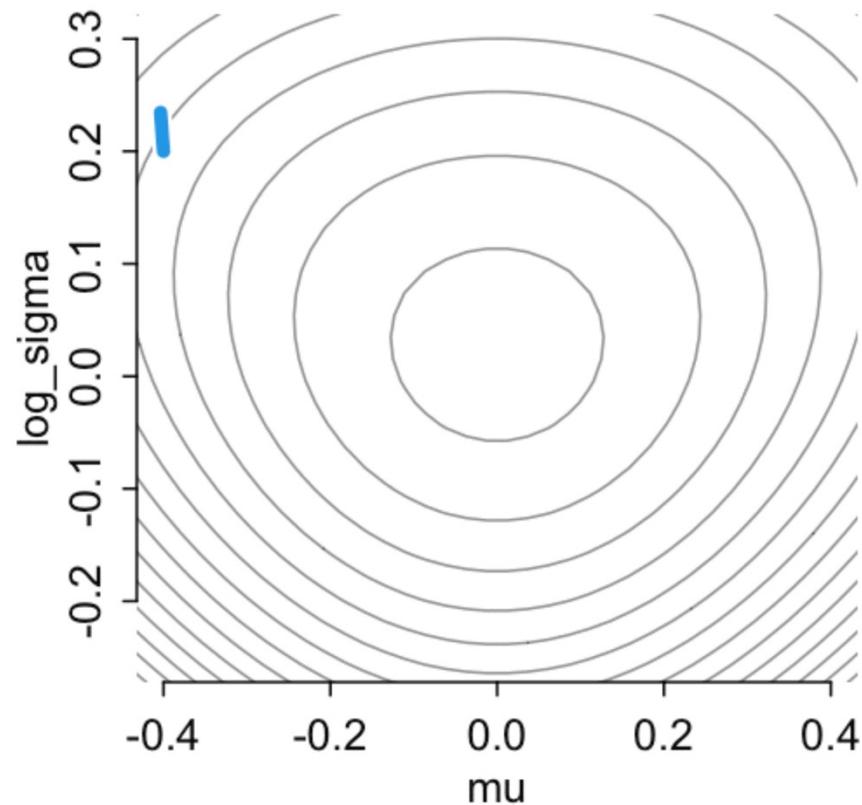
Basic Rosenbluth (aka Metropolis) algorithm



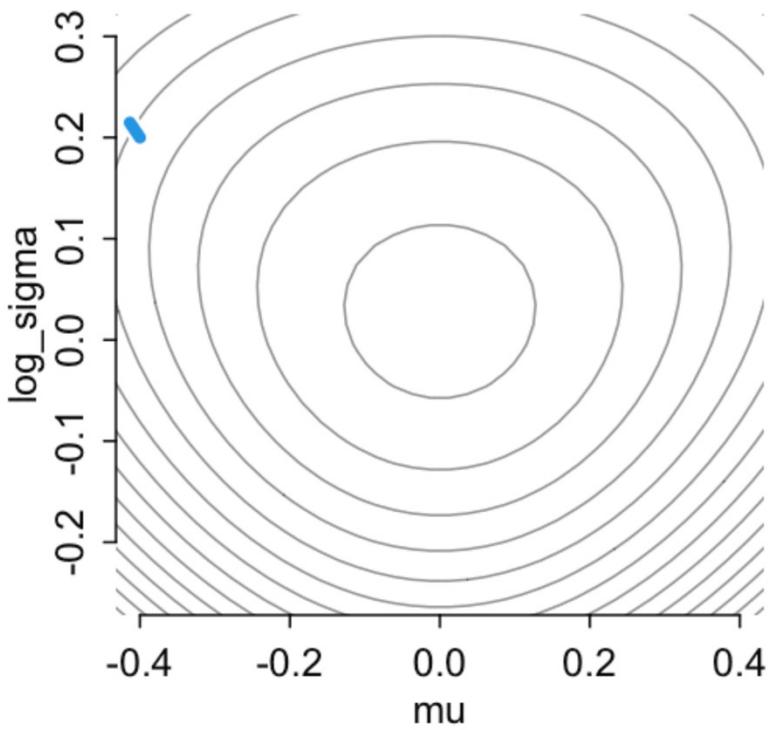
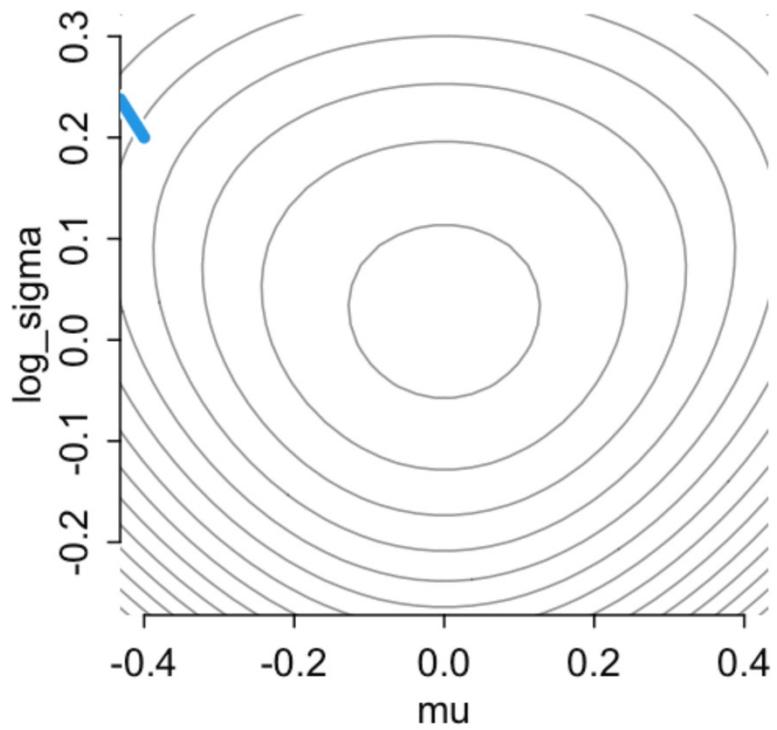
Basic Rosenbluth (aka Metropolis) algorithm

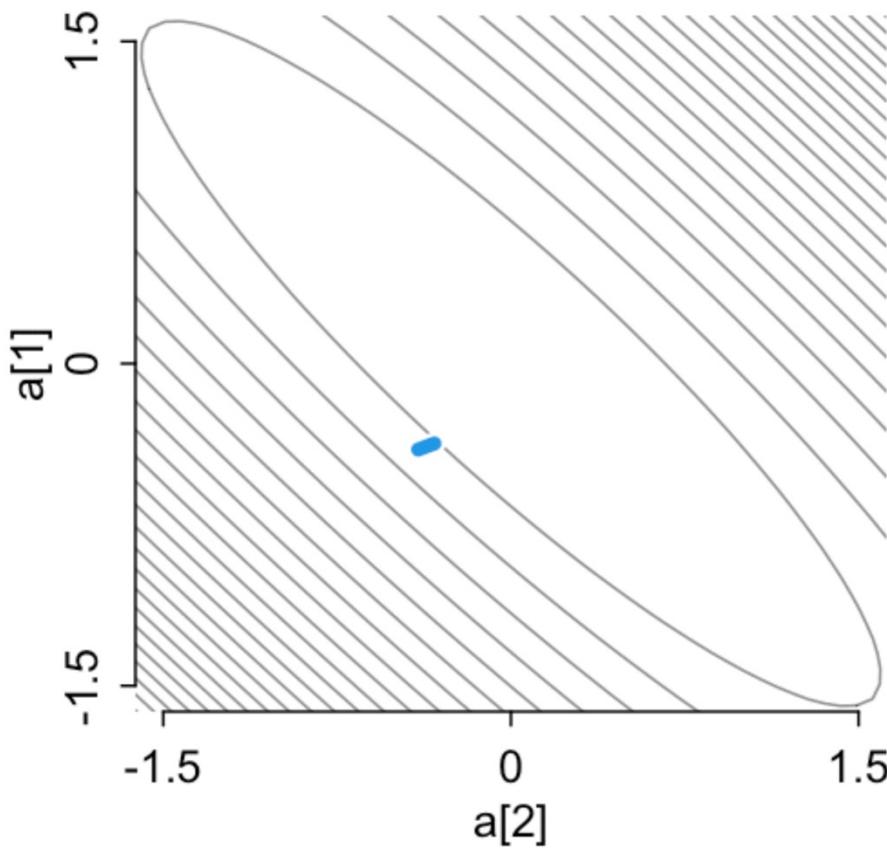


Hamiltonian Monte Carlo



Hamiltonian Monte Carlo





Pages 276–278

276

9. MARKOV CHAIN MONTE CARLO

9.3. HAMILTONIAN MONTE CARLO

277

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 ϵ , (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:

$$\sum_i \log p(y_i | \mu_y, 1) + \sum_i \log p(x_i | \mu_x, 1) + \log p(\mu_y | 0, 0.5) + \log p(\mu_x | 0, 0.5)$$

So it's just four calls to `dnorm` really:

```
R code 9.5
# 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) ) +
    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:

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

And the gradient for μ_y has the same form. Now in code form:

```
R code 9.6
# 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 <- 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))
y <- as.numeric(scale(y))
```

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](#):

```
R code 9.7
library(shape) # for fancy arrows
Q <- list()
Q$yq <- c(-0.1,0.2)
pr <- 0.3
plot( NULL , ylab="muy" , xlab="mux" , xlim=c(-pr,pr) , ylim=c(-pr,pr) )
step <- 0.03
L <- 11 # 0.03/28 for U-turns --- 11 for working example
n_samples <- 4
path_col <- col.alpha("black",0.5)
points( Q$yq[1] , Q$yq[2] , pch=4 , col="black" )
for ( i in 1:n_samples ) {
  Q <- HMC2( U , U.gradient , step , L , Q$yq )
  if ( n_samples < 10 ) {
    for ( j in 1:L ) {
      K0 <- sum(Q$traj[j,]^2)/2 # kinetic energy
      lines( Q$traj[j:(j+1),1] , Q$traj[j:(j+1),2] , col=path_col , lwd=1+2*K0 )
    }
    points( Q$traj[1:L+1,1] , 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.

```
R code 9.8
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))
  ptraj <- qtraj
  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.

```
R code 9.9
# 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
  }
}
```

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

$$J = \begin{bmatrix} \frac{\partial B_x}{\partial x} & \frac{\partial B_y}{\partial x} & \frac{\partial B_z}{\partial x} \\ \frac{\partial B_x}{\partial y} & \frac{\partial B_y}{\partial y} & \frac{\partial B_z}{\partial y} \\ \frac{\partial B_x}{\partial z} & \frac{\partial B_y}{\partial z} & \frac{\partial B_z}{\partial z} \end{bmatrix}$$

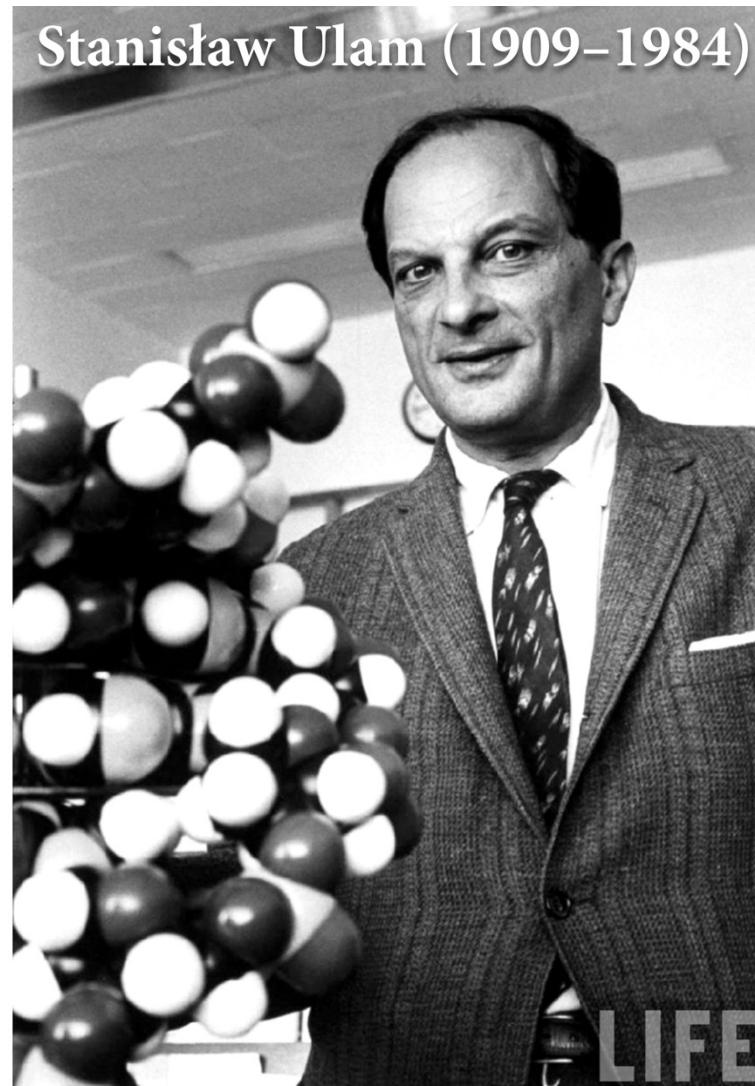

mc-stan.org



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 )
```

$$D_i \sim \text{Normal}(\mu_i, \sigma)$$

$$\mu_i = \alpha + \beta_M M_i + \beta_A A_i$$

$$\alpha \sim \text{Normal}(0,0.2)$$

$$\beta_M \sim \text{Normal}(0,0.5)$$

$$\beta_A \sim \text{Normal}(0,0.5)$$

$$\sigma \sim \text{Exponential}(1)$$

Example: Divorce data

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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 )
library(cmdstanr)
mHMC <- ulam( f , data=dat )
```

$$D_i \sim \text{Normal}(\mu_i, \sigma)$$

$$\mu_i = \alpha + \beta_M M_i + \beta_A A_i$$

$$\alpha \sim \text{Normal}(0,0.2)$$

$$\beta_M \sim \text{Normal}(0,0.5)$$

$$\beta_A \sim \text{Normal}(0,0.5)$$

$$\sigma \sim \text{Exponential}(1)$$

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  0.99  1504    1
mq >
```

```
library(cmdstanr)
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 ~ 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 );
}
```

```
// stan code (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{
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    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

```

// stan code(mHMC)
data{
    // the observed variables
    vector[50] D;
    vector[50] A;
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}
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    bM ~ normal( 0 , 0.5 );
    a ~ normal( 0 , 0.2 );
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    }
    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.

```

// stan code (mHMC)
data{
    // the observed variables
    vector[50] D;
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}
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    real a;
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    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

Pure Stan approach

Save Stan code as own file

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

Extract samples and
proceed as usual

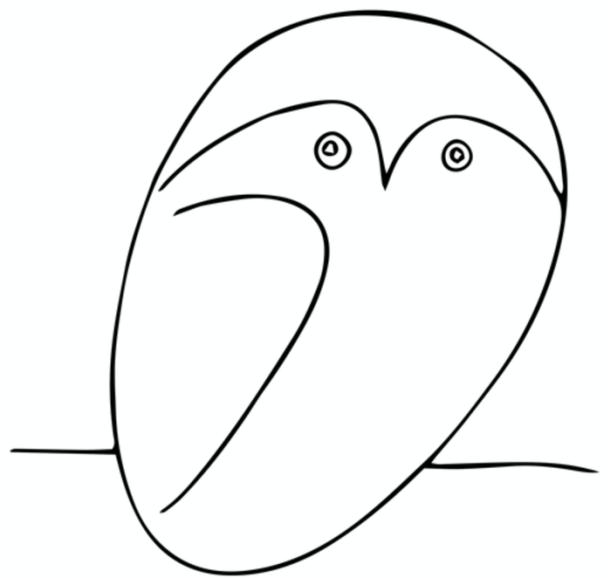
```
post <- extract.samples(mHMC_stan)
```

```
// 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 );  
}
```

Drawing the Markov Owl

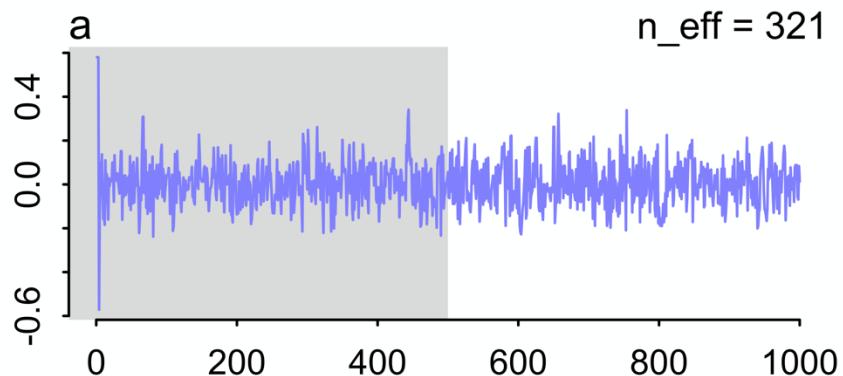
Complex machinery, but lots of diagnostics

- (1) Trace plots
- (2) Trace rank plots
- (3) R-hat convergence measure
- (4) Number of effective samples
- (5) Divergent transitions

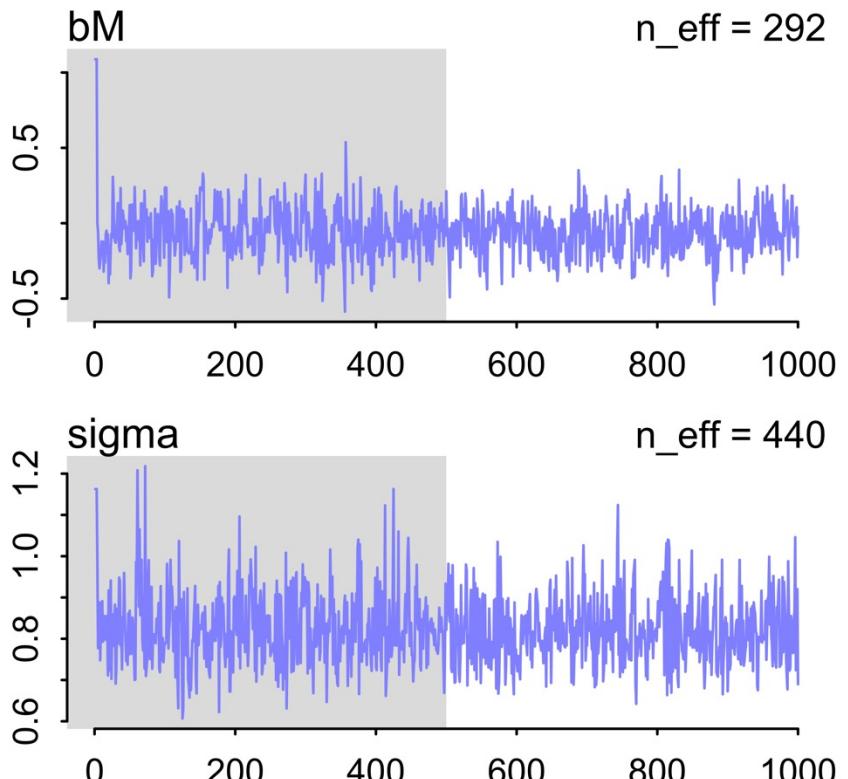
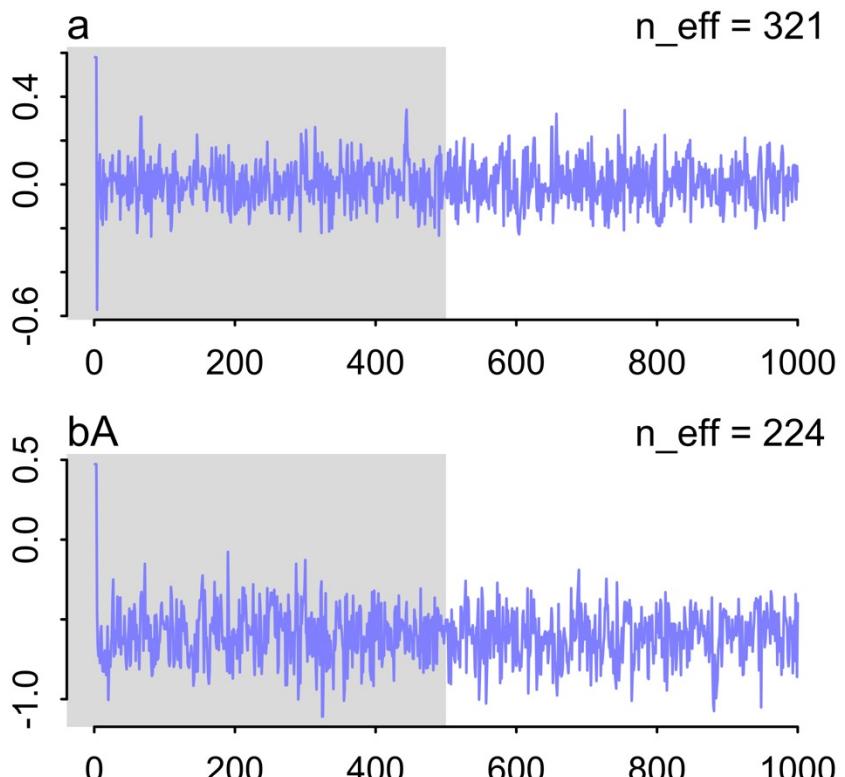


Picasso

Trace plots



Trace plots



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 )

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

$$D_i \sim \text{Normal}(\mu_i, \sigma)$$

$$\mu_i = \alpha + \beta_M M_i + \beta_A A_i$$

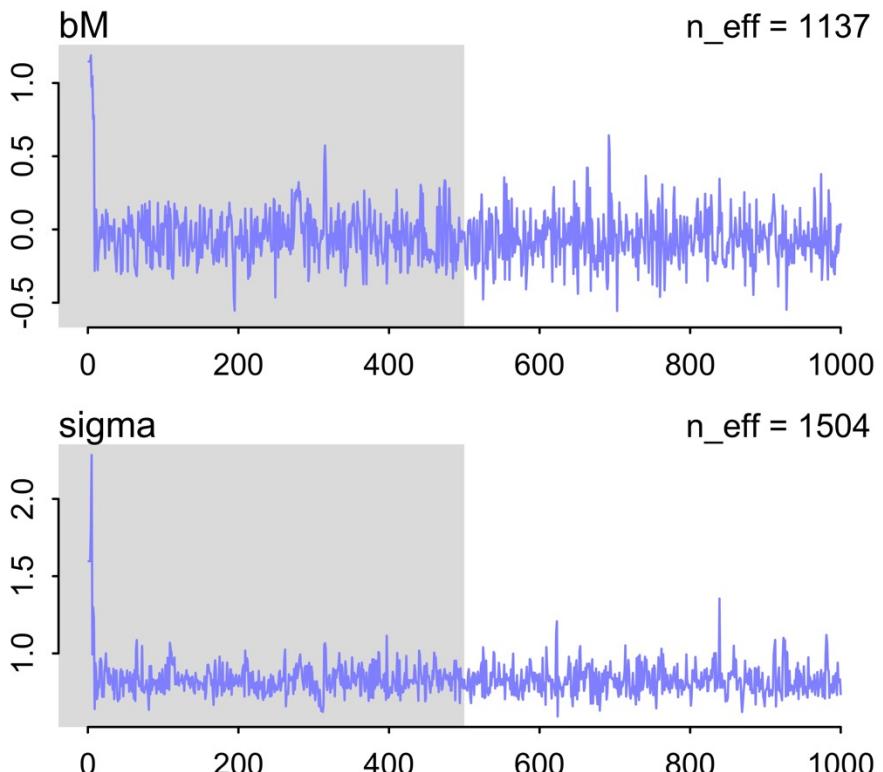
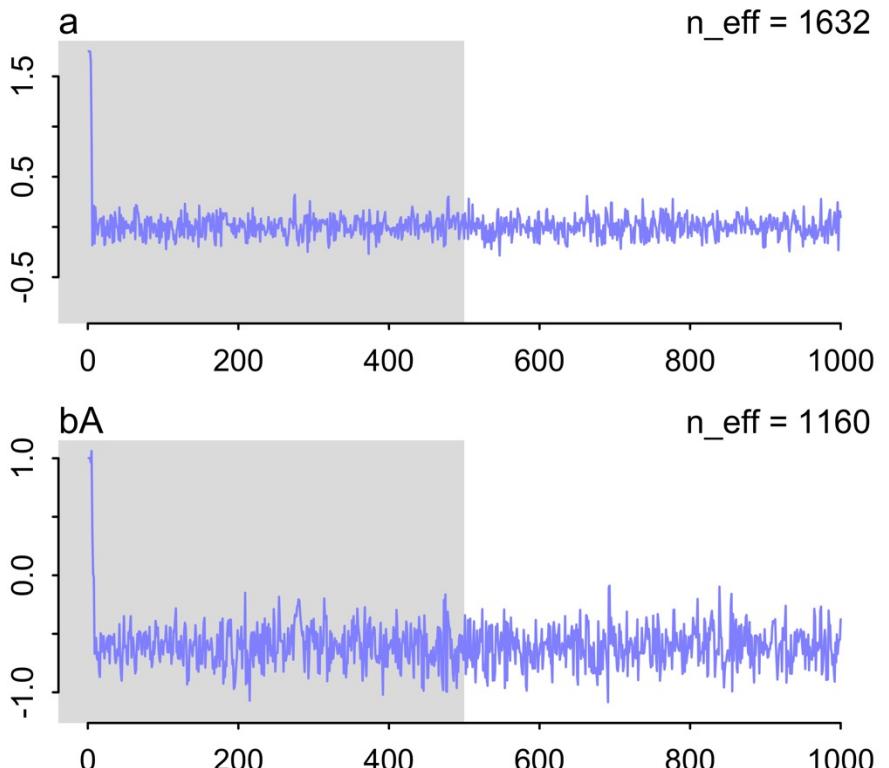
$$\alpha \sim \text{Normal}(0,0.2)$$

$$\beta_M \sim \text{Normal}(0,0.5)$$

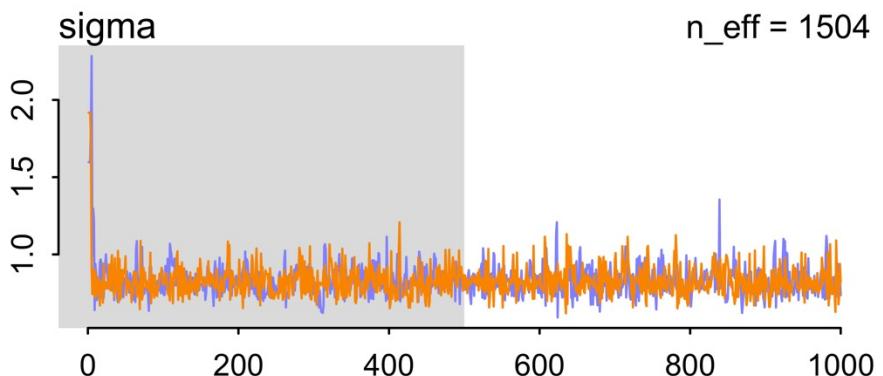
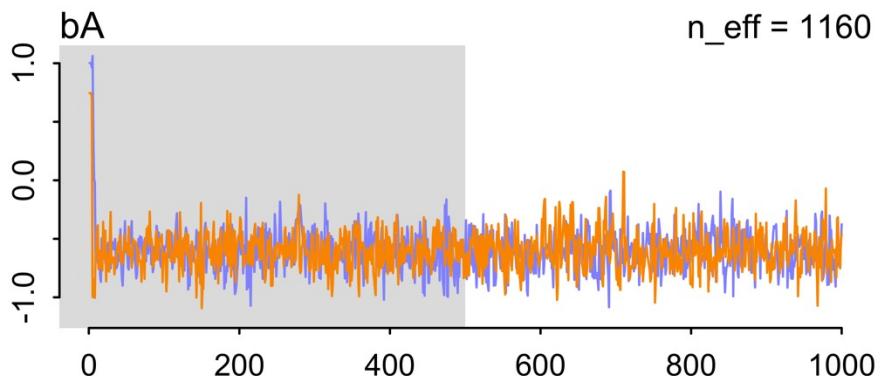
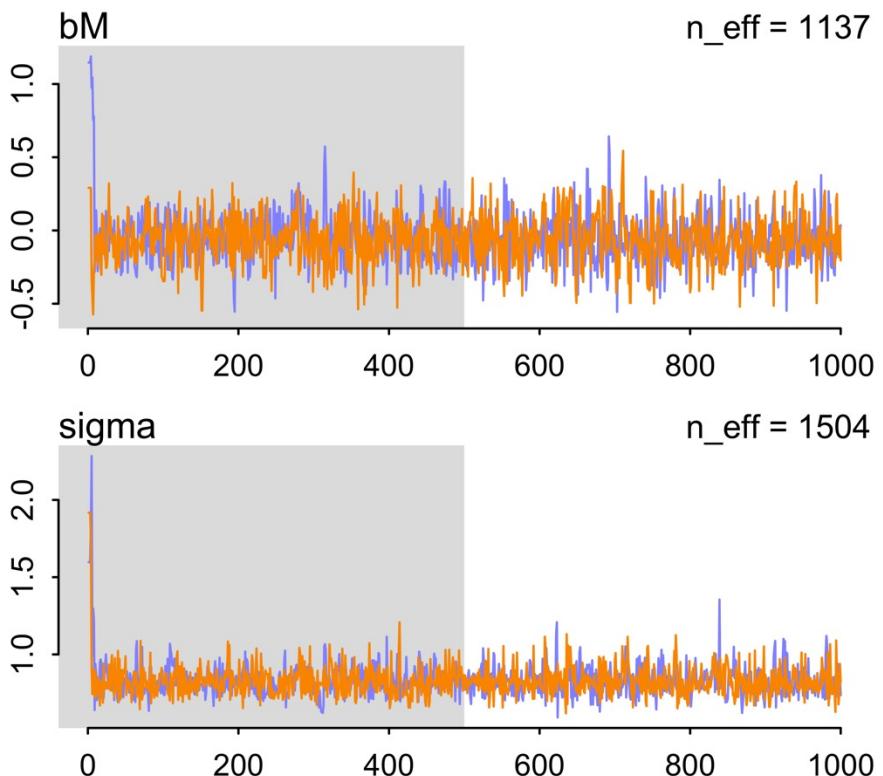
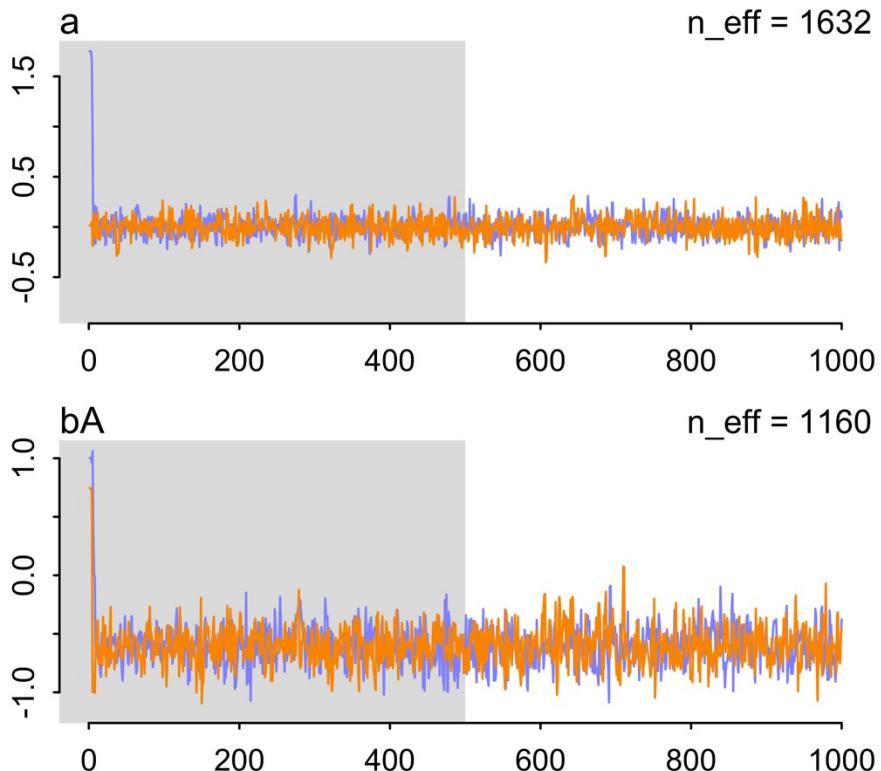
$$\beta_A \sim \text{Normal}(0,0.5)$$

$$\sigma \sim \text{Exponential}(1)$$

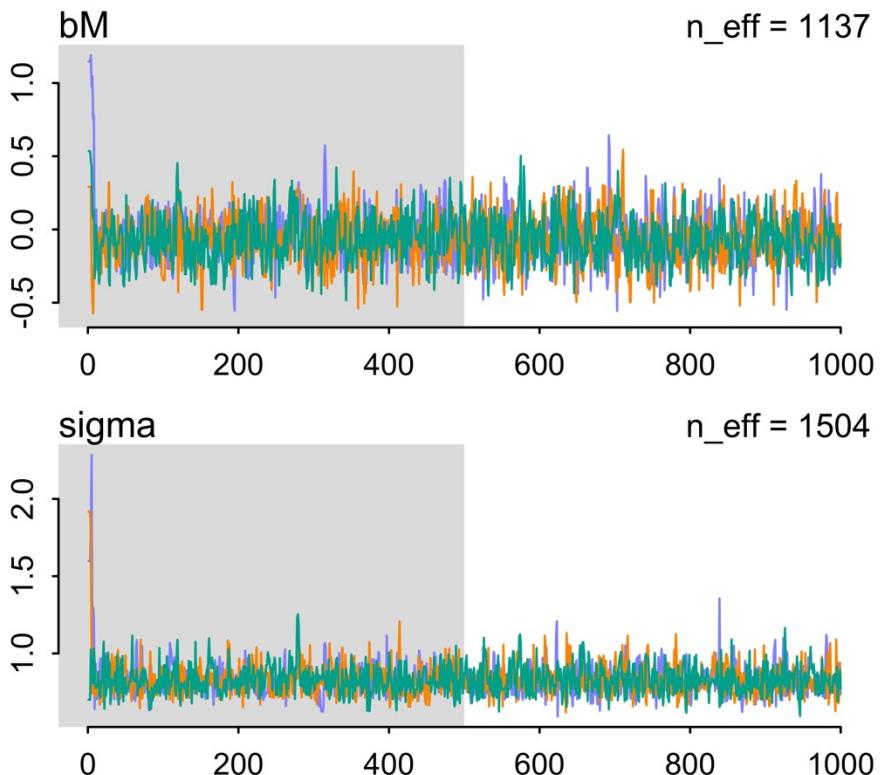
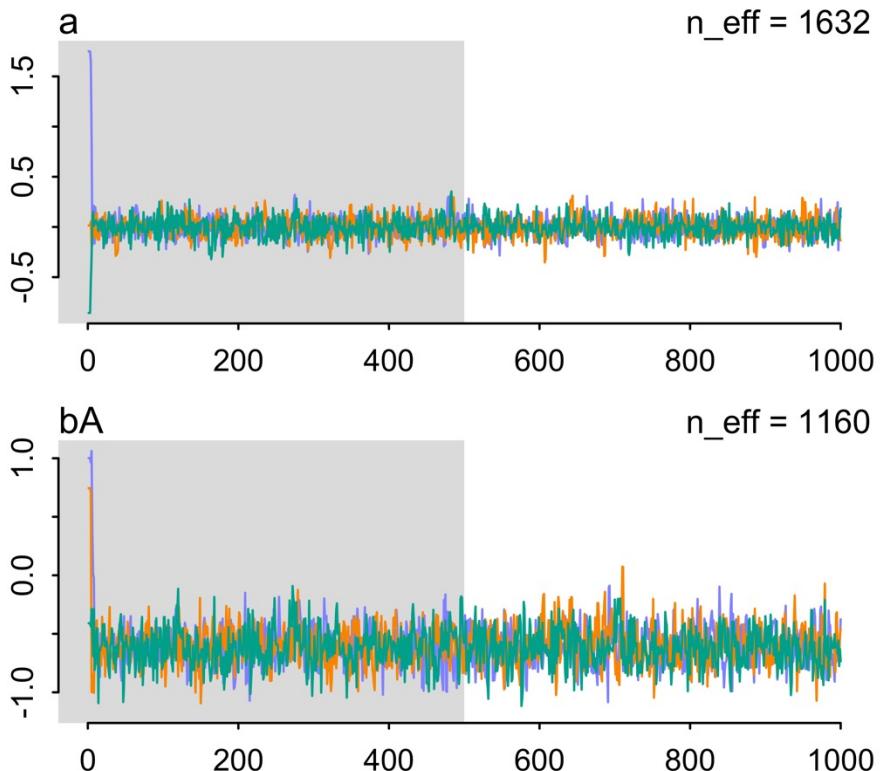
Trace plots



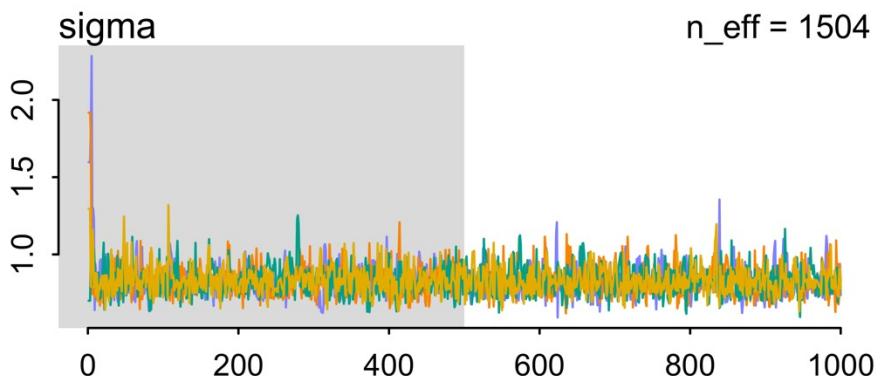
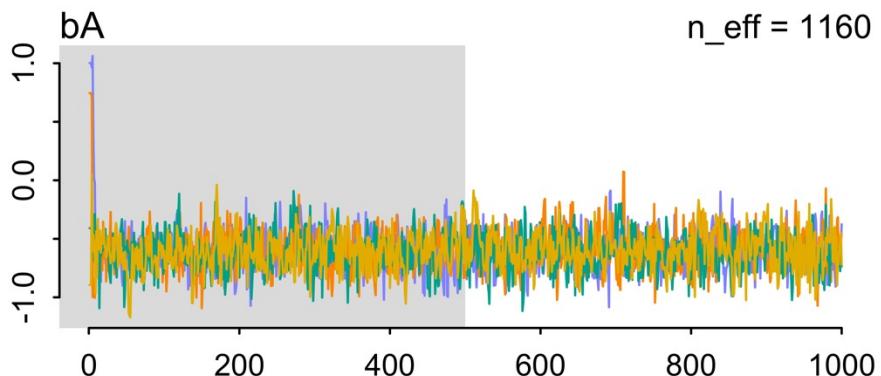
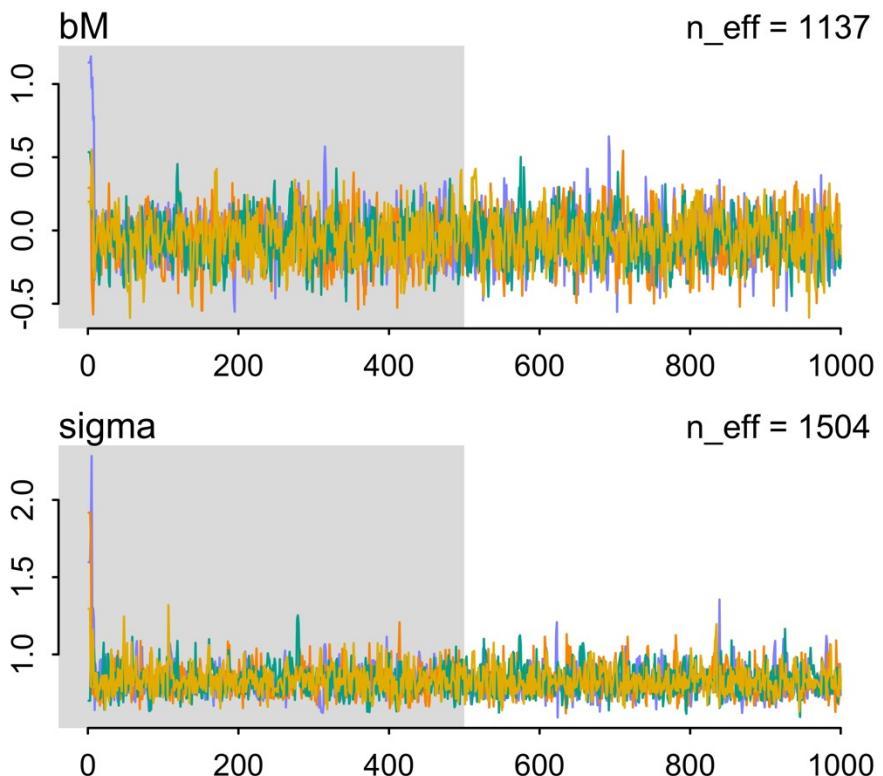
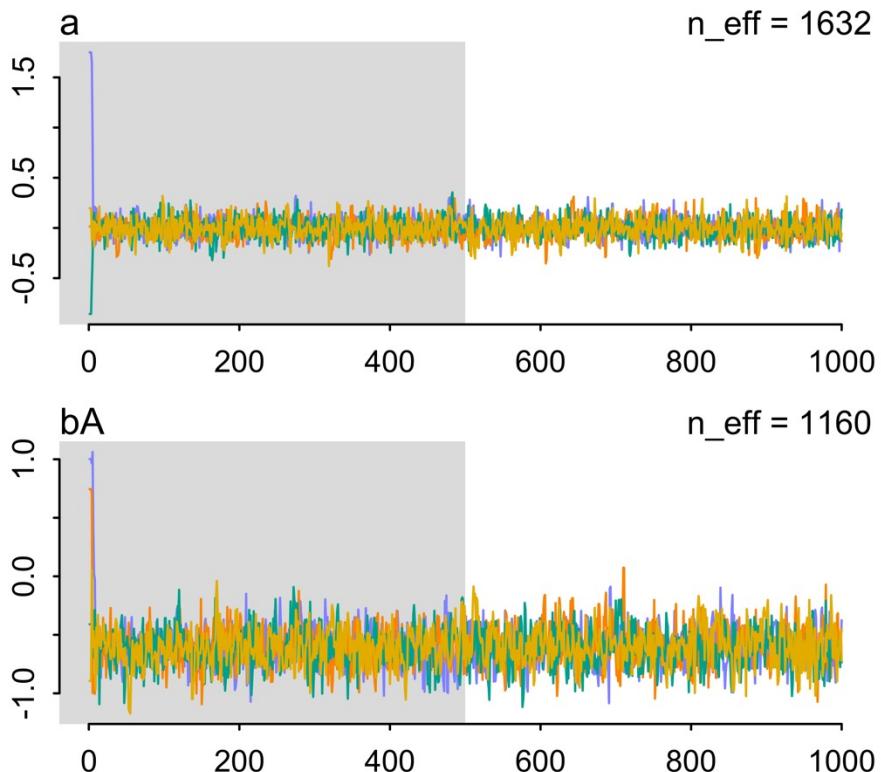
Trace plots



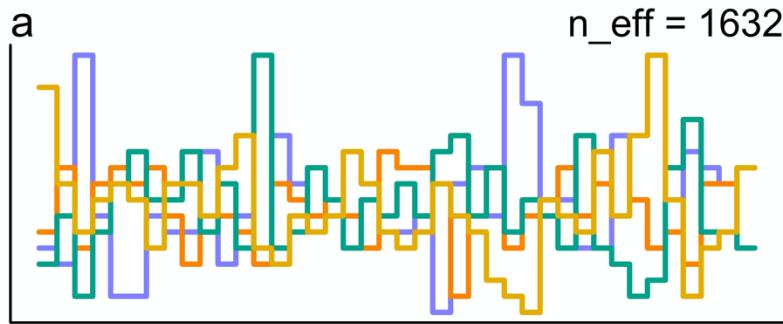
Trace plots



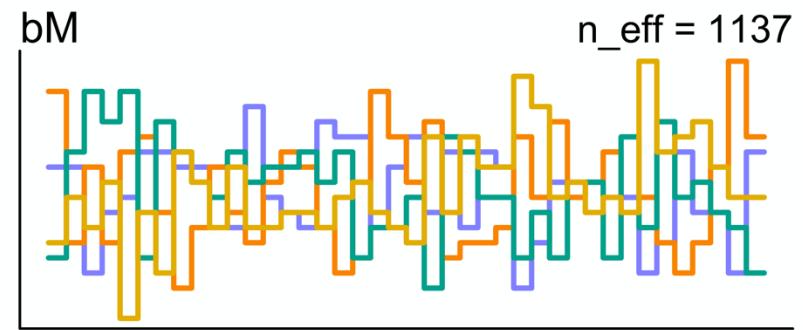
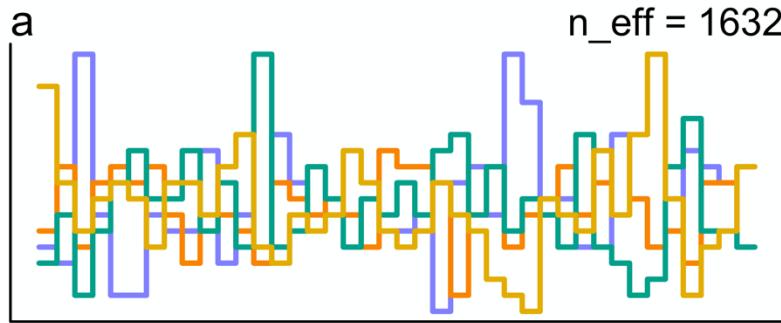
Trace plots



Trace rank (Trank) plots



Trace rank (Trank) plots



R-hat

When chains converge:

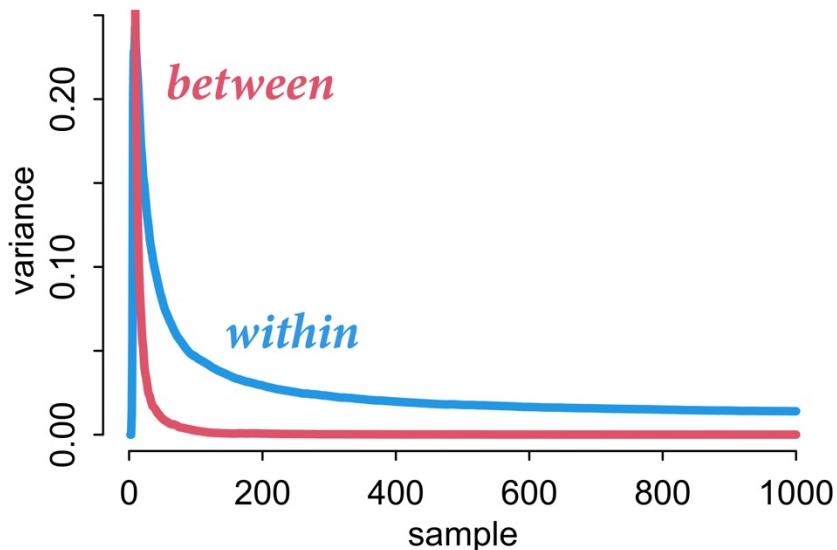
- (1) Start and end of each chain explores same region
- (2) Independent chains explore same region

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

```
> 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
> █
```



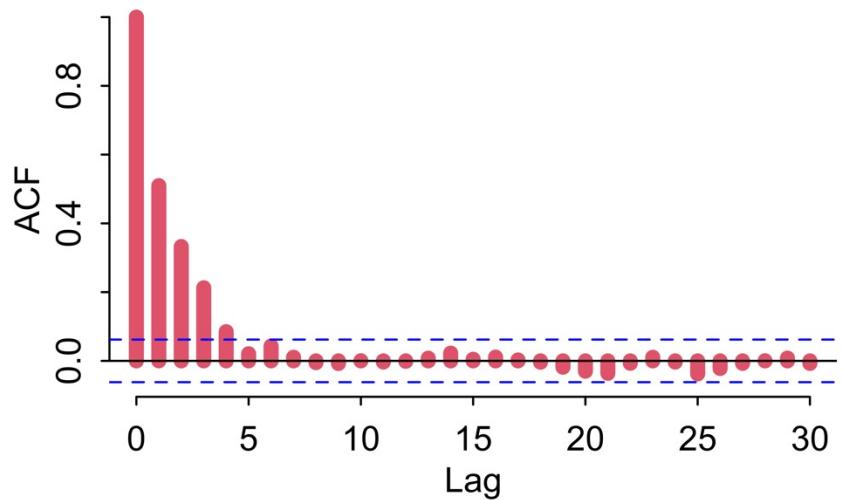
n_eff

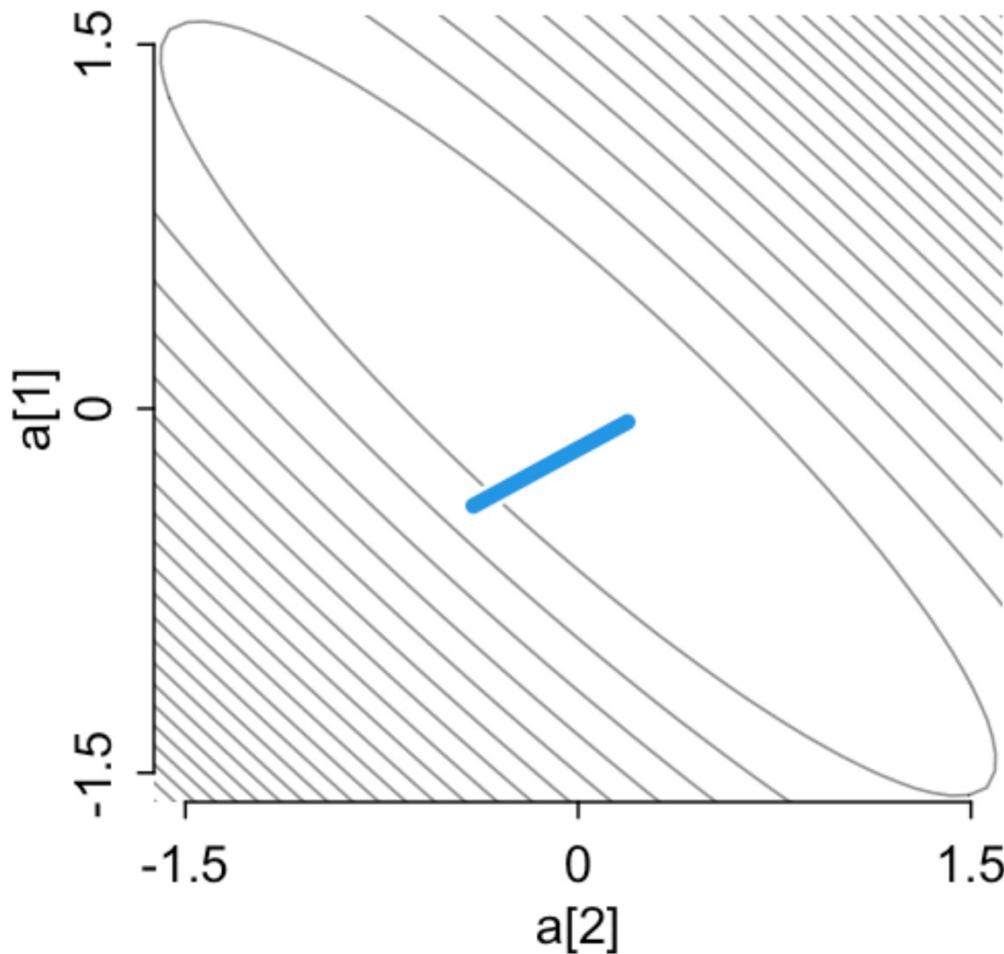
Estimate of number of **effective samples**

“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

```
> 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
>
```





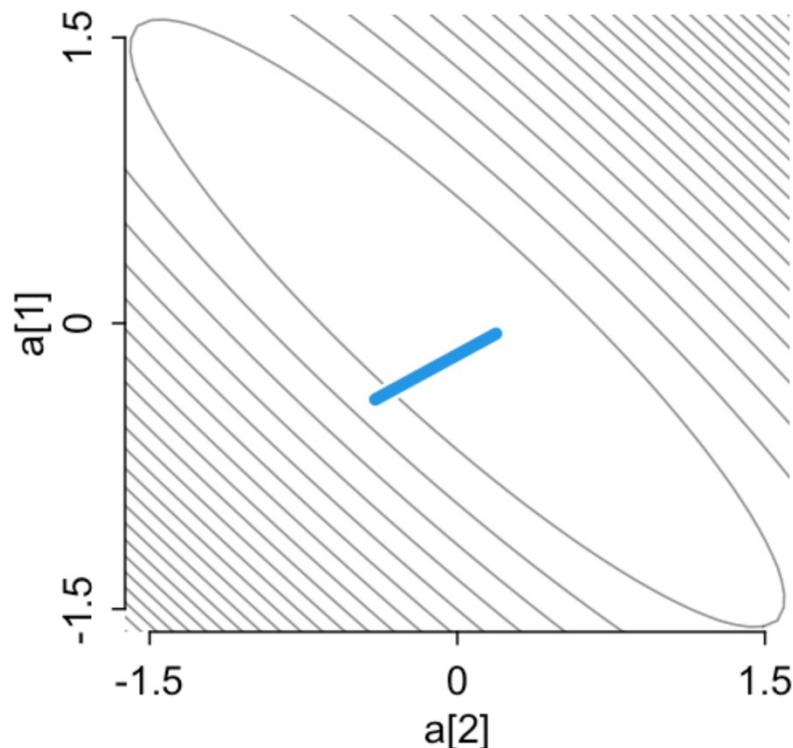
Divergent transitions

Divergent transition: A kind of rejected proposal

Simulation *diverges* from true path

Many DTs: poor exploration & possible bias

Will discuss again in later lecture



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 )
```

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 )
```

```
|> precis(m9.2)
      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
|> |
```

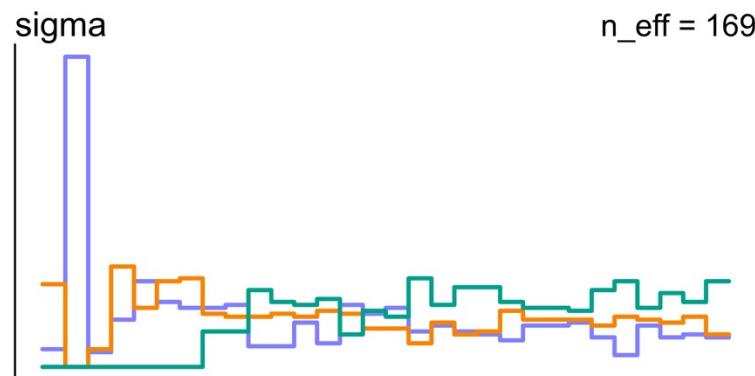
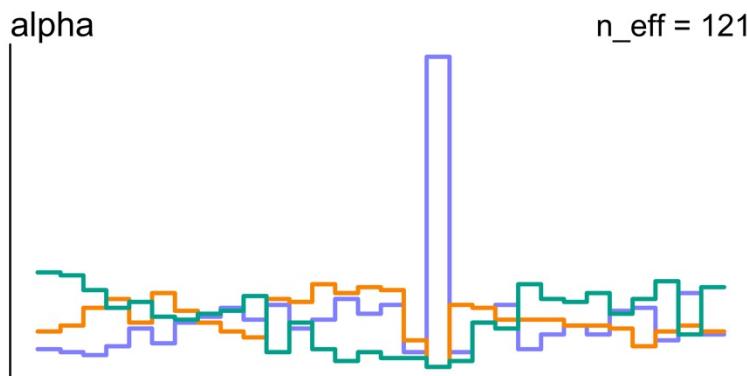
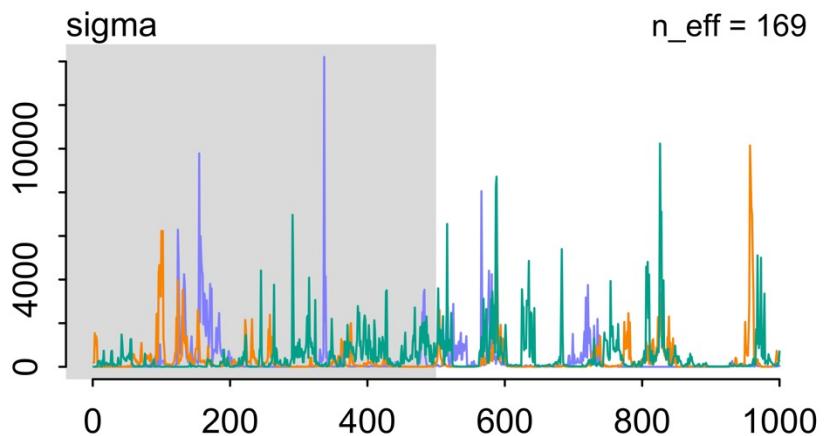
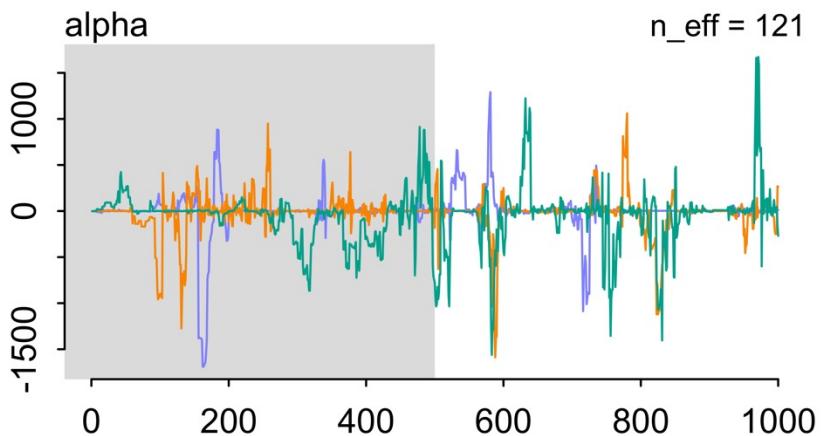
Bad chains

```
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 )
```

```
|> precis(m9.2)
      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
|>
```

Warning: 108 of 1500 (7.0%) transitions ended with a divergence.
This may indicate insufficient exploration of the posterior distribution.
Possible remedies include:

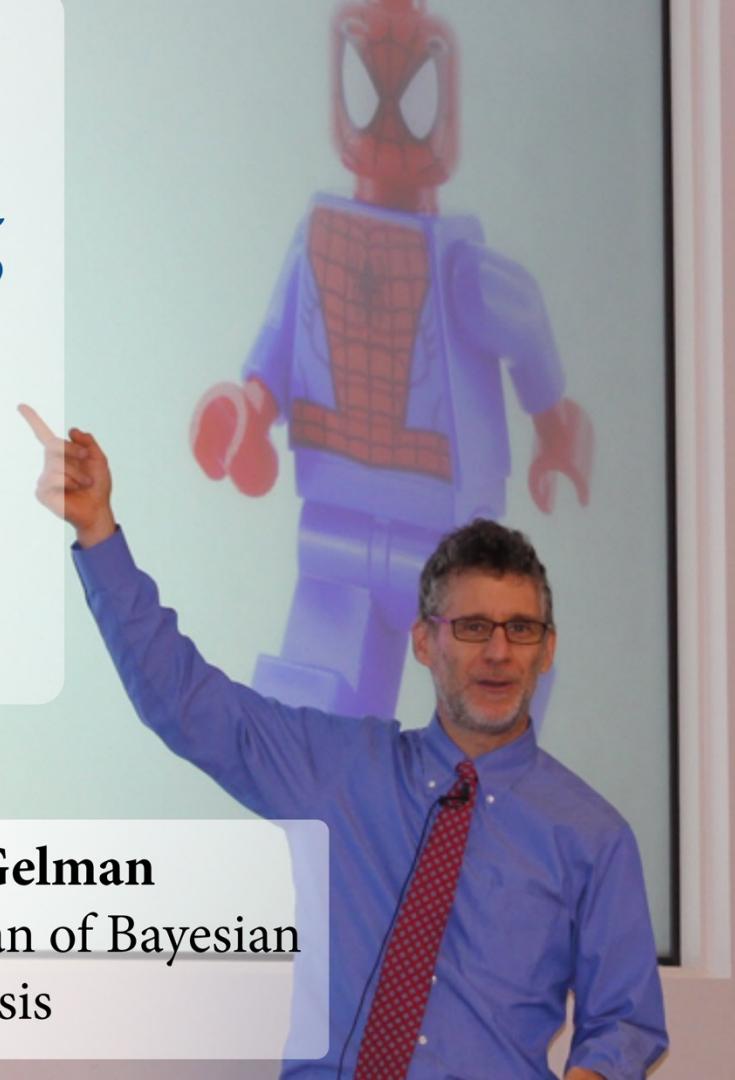
- * Increasing `adapt_delta` closer to 1 (default is 0.8)
- * Reparameterizing the model (e.g. using a non-centered parameterization)
- * Using informative or weakly informative prior distributions



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



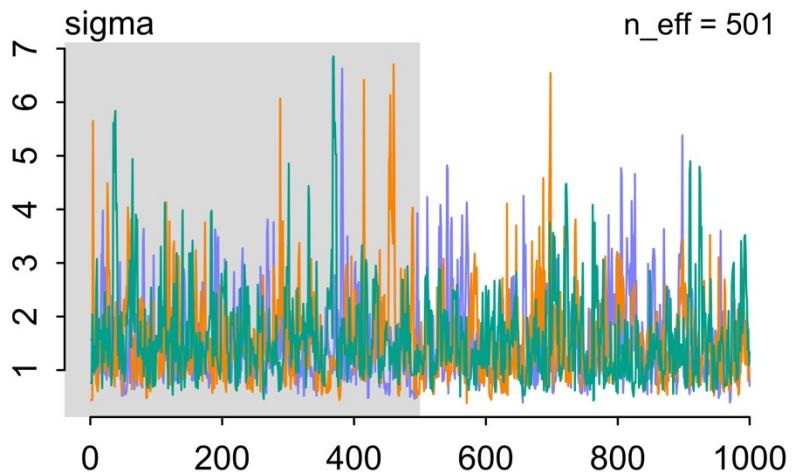
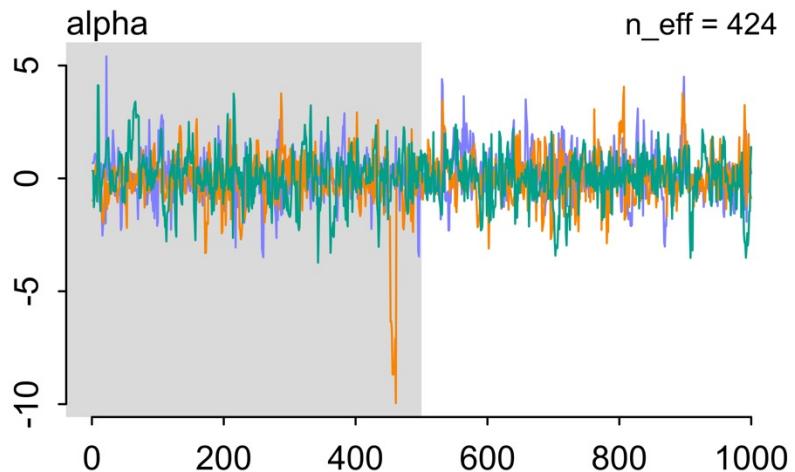
Bad chains

```
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 )
```

```
> precis(m9.2)
      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
>
```

```
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 )
```

```
> precis(m9.3)
      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

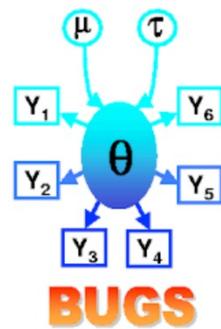
Desktop MCMC has been a revolution in scientific computing

Custom scientific modeling

High-dimension

Propagate measurement error

Do not “pipette by mouth”



Sir David Spiegelhalter