Metropolis-Hastings algorithm

Dr. Jarad Niemi

STAT 544 - Iowa State University

March 28, 2017

Outline

- Metropolis-Hastings algorithm
- Independence proposal
- Random-walk proposal
  - Optimal tuning parameter
  - Binomial example
  - Normal example
  - Binomial hierarchical example

Metropolis-Hastings algorithm

Let

- $p(\theta|y)$ be the target distribution and
- $\theta^{(t)}$ be the current draw from $p(\theta|y)$.

The Metropolis-Hastings algorithm performs the following

1. propose $\theta^* \sim g(\theta|\theta^{(t)})$
2. accept $\theta^{(t+1)} = \theta^*$ with probability $\min\{1, r\}$ where

$$r = r(\theta^{(t)}, \theta^*) = \frac{p(\theta^*|y)/g(\theta^*|\theta^{(t)})}{p(\theta^{(t)}|y)/g(\theta^{(t)}|\theta^*)} = \frac{p(\theta^*|y)}{p(\theta^{(t)}|y)}\frac{g(\theta^{(t)}|\theta^*)}{g(\theta^*|\theta^{(t)})}$$

   otherwise, set $\theta^{(t+1)} = \theta^{(t)}$.

Metropolis-Hastings algorithm

Suppose we only know the target up to a normalizing constant, i.e.

$$p(\theta|y) = q(\theta|y)/p(y)$$

where we only know $q(\theta|y)$.

The Metropolis-Hastings algorithm performs the following

1. propose $\theta^* \sim g(\theta|\theta^{(t)})$
2. accept $\theta^{(t+1)} = \theta^*$ with probability $\min\{1, r\}$ where

$$r = r(\theta^{(t)}, \theta^*) = \frac{p(\theta^*|y)}{p(\theta^{(t)}|y)} \frac{g(\theta^{(t)}|\theta^*)}{g(\theta^*|\theta^{(t)})} = \frac{q(\theta^*|y)/p(y)}{q(\theta^{(t)}|y)/p(y)} \frac{g(\theta^{(t)}|\theta^*)}{g(\theta^*|\theta^{(t)})} = \frac{q(\theta^*|y)}{q(\theta^{(t)}|y)} \frac{g(\theta^{(t)}|\theta^*)}{g(\theta^*|\theta^{(t)})}$$

otherwise, set $\theta^{(t+1)} = \theta^{(t)}$.

Two standard Metropolis-Hastings algorithms

- Independent Metropolis-Hastings
  - Independent proposal, i.e. $g(\theta|\theta^{(t)}) = g(\theta)$
- Random-walk Metropolis
  - Symmetric proposal, i.e. $g(\theta|\theta^{(t)}) = g(\theta^{(t)}|\theta)$ for all $\theta, \theta^{(t)}$.

Independence Metropolis-Hastings

Let

- $p(\theta|y) \propto q(\theta|y)$ be the target distribution,
- $\theta^{(t)}$ be the current draw from $p(\theta|y)$, and
- $g(\theta|\theta^{(t)}) = g(\theta)$, i.e. the proposal is independent of the current value.

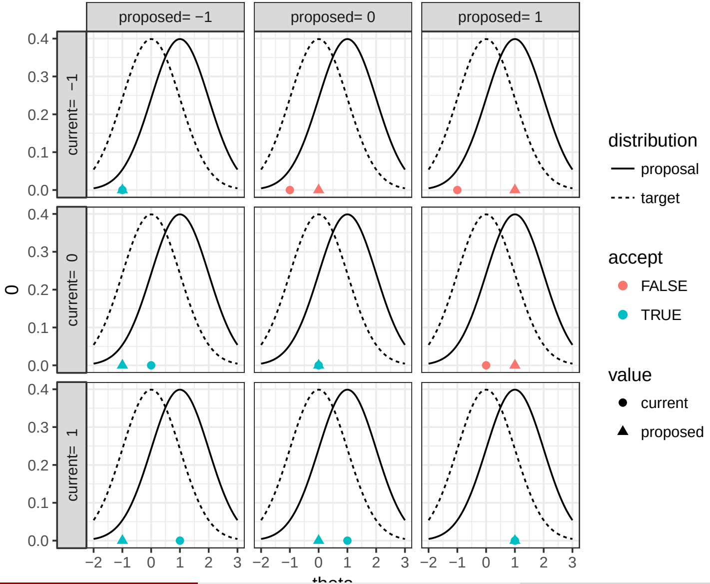
The independence Metropolis-Hastings algorithm performs the following

1. propose $\theta^* \sim g(\theta)$
2. accept $\theta^{(t+1)} = \theta^*$ with probability $\min\{1, r\}$ where

$$r = \frac{q(\theta^*|y)/g(\theta^*)}{q(\theta^{(t)}|y)/g(\theta^{(t)})} = \frac{q(\theta^*|y)}{q(\theta^{(t)}|y)}\frac{g(\theta^{(t)})}{g(\theta^*)}$$

otherwise, set $\theta^{(t+1)} = \theta^{(t)}$.

Intuition through examples



Example: Normal-Cauchy model

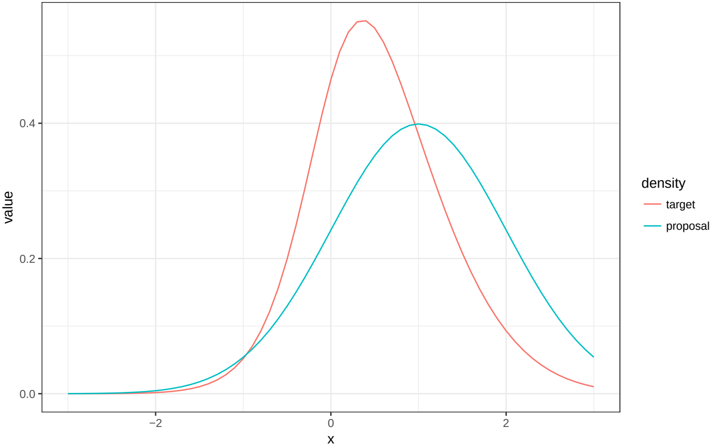
Let $Y \sim N(\theta, 1)$ with $\theta \sim Ca(0,1)$ such that the posterior is

$$p(\theta|y) \propto p(y|\theta)p(\theta) \propto \frac{\exp(-(y-\theta)^2/2)}{1+\theta^2}$$

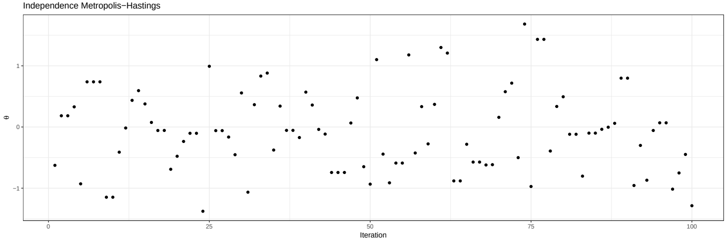
Use $N(y,1)$ as the proposal, then the Metropolis-Hastings acceptance probability is the $\min\{1, r\}$ with

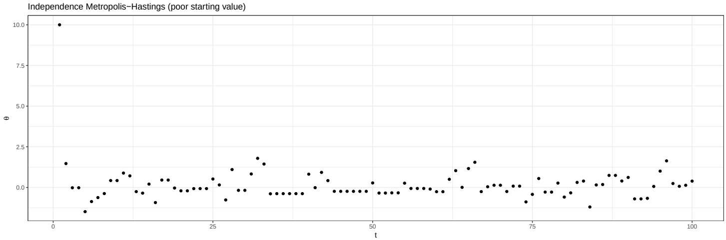
$$\begin{array}{rcl} r &=& \frac{q(\theta^*|y)}{q(\theta^{(t)}|y)} \frac{g(\theta^{(t)})}{g(\theta^*)} \\ &=& \frac{\exp(-(y-\theta^*)^2/2)/1+(\theta^*)^2}{\exp(-(y-\theta^{(t)})^2/2)/1+(\theta^{(t)})^2} \frac{\exp(-(\theta^{(t)}-y)^2/2)}{\exp(-(\theta^*-y)^2/2)} \\ &=& \frac{1+(\theta^{(t)})^2}{1+(\theta^*)^2} \end{array}$$

Example: Normal-Cauchy model



Example: Normal-Cauchy model





Need heavy tails

Recall that

- rejection sampling requires the proposal to have heavy tails and
- importance sampling is efficient only when the proposal has heavy tails.

Independence Metropolis-Hastings also requires heavy tailed proposals for efficiency since if $\theta^{(t)}$ is

- in a region where $p(\theta^{(t)}|y) >> g(\theta^{(t)})$ then
- any proposal θ^* such that $p(\theta^*|y) \approx g(\theta^*)$

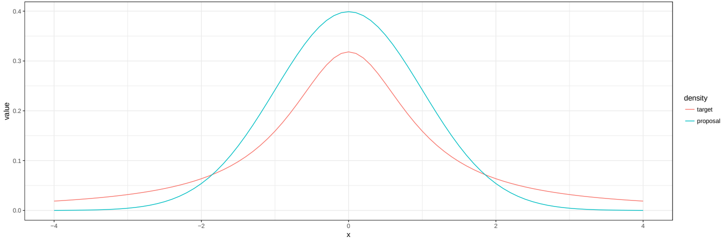
will result in

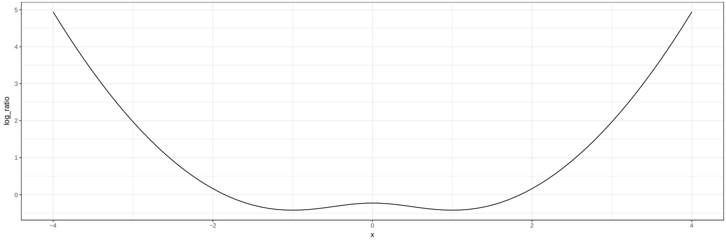
$$r = \frac{g(\theta^{(t)})}{p(\theta^{(t)}|y)} \frac{p(\theta^*|y)}{g(\theta^*)} \approx 0$$

and few samples will be accepted.

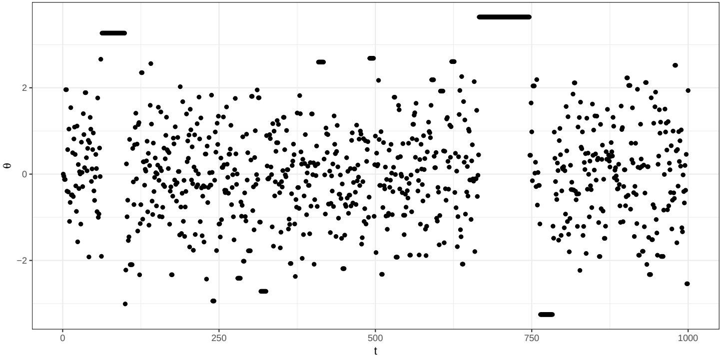
Need heavy tails - example

Suppose $\theta|y \sim Ca(0,1)$ and we use a standard normal as a proposal. Then





Need heavy tails



Random-walk Metropolis

Let

- $p(\theta|y) \propto q(\theta|y)$ be the target distribution,
- $\theta^{(t)}$ be the current draw from $p(\theta|y)$, and
- $g(\theta^*|\theta^{(t)}) = g(\theta^{(t)}|\theta^*)$, i.e. the proposal is symmetric.

The Metropolis algorithm performs the following

1. propose $\theta^* \sim g(\theta|\theta^{(t)})$
2. accept $\theta^{(t+1)} = \theta^*$ with probability $\min\{1, r\}$ where

$$r = \frac{q(\theta^*|y)}{q(\theta^{(t)}|y)} \frac{g(\theta^{(t)}|\theta^*)}{g(\theta^*|\theta^{(t)})} = \frac{q(\theta^*|y)}{q(\theta^{(t)}|y)}$$

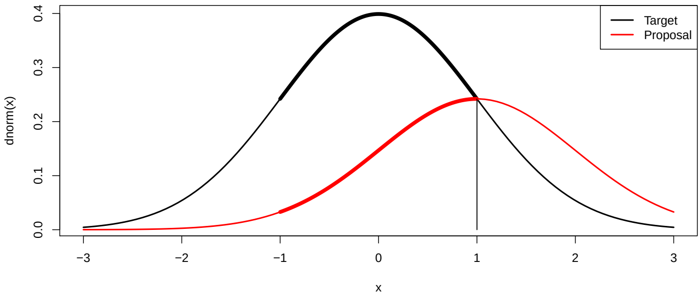
   otherwise, set $\theta^{(t+1)} = \theta^{(t)}$.

This is also referred to as random-walk Metropolis.

Stochastic hill climbing

Notice that $r = q(\theta^*|y)/q(\theta^{(t)}|y)$ and thus will accept whenever the target density is larger when evaluated at the proposed value than it is when evaluated at the current value.

Suppose $\theta|y \sim N(0,1)$, $\theta^{(t)} = 1$, and $\theta^* \sim N(\theta^{(t)}, 1)$.



Example: Normal-Cauchy model

Let $Y \sim N(\theta, 1)$ with $\theta \sim Ca(0,1)$ such that the posterior is

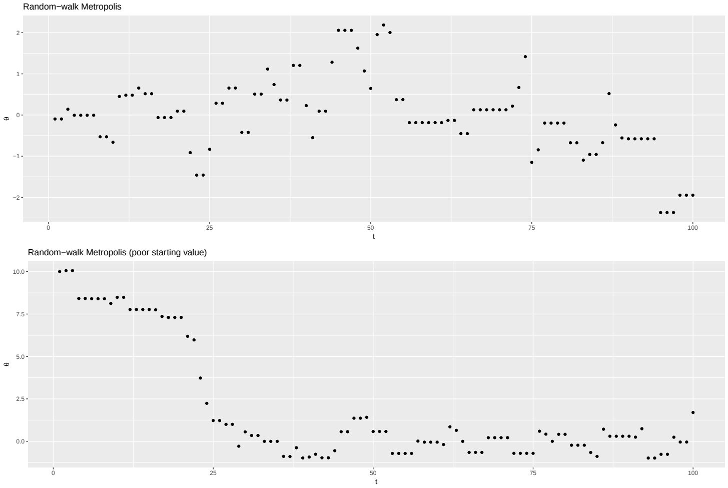
$$p(\theta|y) \propto p(y|\theta)p(\theta) \propto \frac{\exp(-(y-\theta)^2/2)}{1+\theta^2}$$

Use $N(\theta^{(t)}, \tau^2)$ as the proposal, then the acceptance probability is the $\min\{1, r\}$ with

$$r = \frac{q(\theta^*|y)}{q(\theta^{(t)}|y)} = \frac{p(y|\theta^*)p(\theta^*)}{p(y|\theta^{(t)})p(\theta^{(t)})}.$$

For this example, let $\tau^2 = 1$.

Example: Normal-Cauchy model



Random-walk tuning parameter

Let $p(\theta|y)$ be the target distribution, the proposal is symmetric with scale τ^2, and $\theta^{(t)}$ is (approximately) distributed according to $p(\theta|y)$.

- If $\tau^2 \approx 0$, then $\theta^* \approx \theta^{(t)}$ and

$$r = \frac{q(\theta^*|y)}{q(\theta^{(t)}|y)} \approx 1$$

  and all proposals are accepted.

- As $\tau^2 \to \infty$, then $q(\theta^*|y) \approx 0$ since θ^* will be far from the mass of the target distribution and

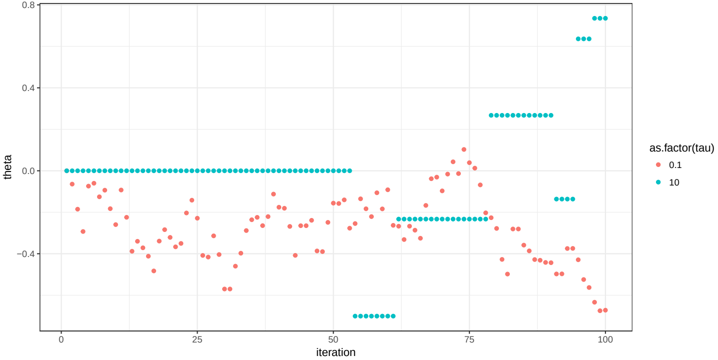
$$r = \frac{q(\theta^*|y)}{q(\theta^{(t)}|y)} \approx 0$$

  so all proposed values are rejected.

So there is an optimal τ^2 somewhere. For normal targets, the optimal random-walk proposal variance is $2.4^2 Var(\theta|y)/d$ where d is the dimension of θ which results in an acceptance rate of 40% for $d = 1$ down to 20% as $d \to \infty$.

Random-walk with tuning parameter that is too big and too small

Let $y|\theta \sim N(\theta, 1)$, $\theta \sim Ca(0,1)$, and $y = 1$.



Binomial model

Let $Y \sim Bin(n, \theta)$ and $\theta \sim Be(1/2, 1/2)$, thus the posterior is

$$p(\theta|y) \propto \theta^{y-0.5}(1-\theta)^{n-y-0.5}\mathrm{I}(0 < \theta < 1).$$

To construct a random-walk Metropolis algorithm, we choose the proposal

$$\theta^* \sim N(\theta^{(t)}, 0.4^2)$$

and accept with probability $\min\{1, r\}$ where

$$r = \frac{p(\theta^*|y)}{p(\theta^{(t)}|y)} = \frac{(\theta^*)^{y-0.5}(1-\theta^*)^{n-y-0.5}\mathrm{I}(0 < \theta^* < 1)}{(\theta^{(t)})^{y-0.5}(1-\theta^{(t)})^{n-y-0.5}\mathrm{I}(0 < \theta^{(t)} < 1)}$$

Binomial model

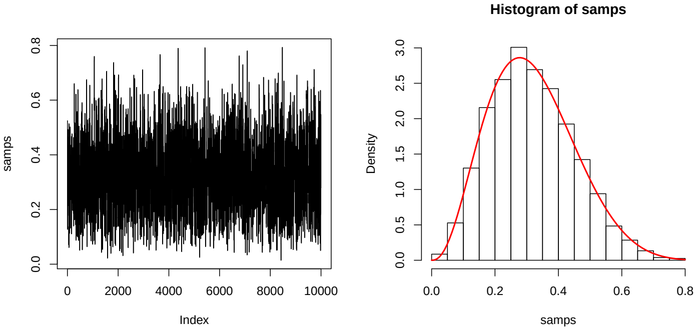
```
n = 10000
log_q = function(theta, y=3, n=10) {
  if (theta<0 | theta>1) return(-Inf)
  (y-0.5)*log(theta)+(n-y-0.5)*log(1-theta)
}
current = 0.5     # Initial value
samps = rep(NA,n)
for (i in 1:n) {
  proposed = rnorm(1, current, 0.4) # tuning parameter is 0.4

  logr = log_q(proposed)-log_q(current)
  if (log(runif(1)) < logr) current = proposed

  samps[i] = current
}
length(unique(samps))/n # acceptance rate

[1] 0.3746
```

Binomial


samps
0.0
0.2
0.4
0.6
0.8
0
2000
4000
6000
8000
10000
Index
Histogram of samps
Density
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0.0
0.2
0.4
0.6
0.8
samps

Normal model

Assume

$$Y_i \stackrel{ind}{\sim} N(\mu, \sigma^2) \qquad \text{and} \qquad p(\mu, \sigma) \propto Ca^+(\sigma; 0, 1)$$

and thus

$$\begin{aligned} p(\mu, \sigma|y) &\propto \left[\prod_{i=1}^n \sigma^{-1} \exp\left(-\tfrac{1}{2\sigma^2}(y_i - \mu)^2\right)\right] \tfrac{1}{1+\sigma^2} \mathrm{I}(\sigma > 0) \\ &= \sigma^{-n} \exp\left(-\tfrac{1}{2\sigma^2}\left[\sum_{i=1}^n y_i^2 - 2\mu n \overline{y} + \mu^2\right]\right) \tfrac{1}{1+\sigma^2} \mathrm{I}(\sigma > 0) \end{aligned}$$

Perform a random-walk Metropolis using a normal proposal, i.e. if $\mu^{(t)}$ and $\sigma^{(t)}$ are the current values for μ and σ, then

$$\left(\begin{array}{c} \mu^* \\ \sigma^* \end{array}\right) \sim N\left(\left[\begin{array}{c} \mu^{(t)} \\ \sigma^{(t)} \end{array}\right], \Sigma\right)$$

where Σ is the tuning parameter.

Adapting the tuning parameter

Recall that the optimal random-walk tuning parameter (if the target is normal) is $2.4^2 Var(\theta|y)/d$ where $Var(\theta|y)$ is the unknown posterior covariance matrix. We can estimate $Var(\theta|y)$ using the sample covariance matrix of draws from the posterior.

Proposed automatic adapting of the Metropolis-Hastings tuning parameter:

1. Start with Σ_0. Set $b = 0$.
2. Run M iterations of the MCMC using $2.4^2\Sigma_b/d$.
3. Set Σ_{b+1} to the sample covariance matrix of all previous draws.
4. If $b < B$, set $b = b + 1$ and return to step 2. Otherwise, throw away all previous draws and go to step 5.
5. Run K iterations of the MCMC using $2.4^2\Sigma_B/d$.

R code for Metropolis-Hastings

```
n = 20
y = rnorm(n)
sum_y2 = sum(y^2)
nybar  = mean(y)
log_q = function(x) {
  if (x[2]<0) return(-Inf)
  -n*log(x[2])-(sum_y2-2*nybar*x[1]+n*x[1]^2)/(2*x[2]^2)-log(1+x[2]^2)
}

B = 10
M = 100

samps = matrix(NA, nrow=B*M, ncol=2)
a_rate = rep(NA, B)

# Initialize
Sigma = diag(2)  # Sigma_0
current = c(0,1)
```

R code for Metropolis-Hastings - Adapting

```
# Adapt
for (b in 1:B) {
  for (m in 1:M) {
    i = (b-1)*M+m

    proposed = mvrnorm(1, current, 2.4^2*Sigma/2)

    logr = log_q(proposed) - log_q(current)
    if (log(runif(1)) < logr) current = proposed
    samps[i,] = current
  }
  a_rate[b] = length(unique(samps[1:i,1]))/length(samps[1:i,1])
  Sigma = var(samps[1:i,])
}
a_rate
```

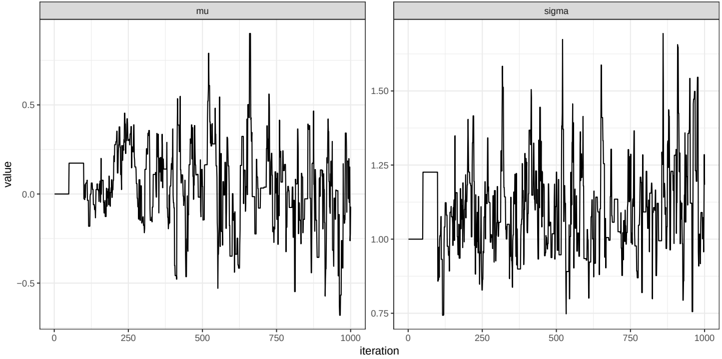
```
 [1] 0.0300000 0.2700000 0.3566667 0.4000000 0.4240000 0.4333333 0.4200000 0.4175000 0.4166667 0.4270000
```

```
var(samps) # Sigma_B
```

```
           [,1]       [,2]
[1,] 0.04898222 0.00255292
[2,] 0.00255292 0.02365873
```

R code for Metropolis-Hastings - Adapting

```
samps = as.data.frame(samps); names(samps) = c("mu","sigma"); samps$iteration = 1:nrow(samps)
ggplot(melt(samps, id.var='iteration', variable.name='parameter'), aes(x=iteration, y=value)) +
  geom_line() +
  facet_wrap(~parameter, scales='free')+
  theme_bw()
```



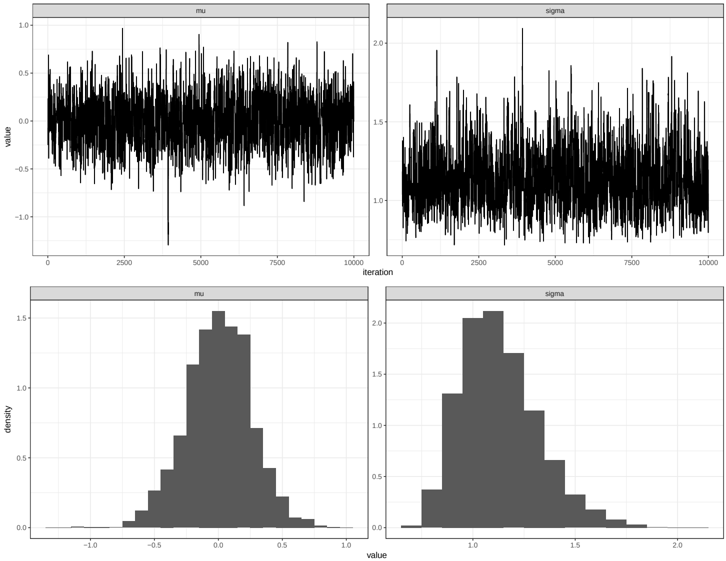
R code for Metropolis-Hastings - Inference

```
# Final run
K = 10000
samps = matrix(NA, nrow=K, ncol=2)
for (k in 1:K) {
  proposed = mvrnorm(1, current, 2.4^2*Sigma/2)

  logr = log_q(proposed) - log_q(current)
  if (log(runif(1)) < logr) current = proposed
  samps[k,] = current
}
length(unique(na.omit(samps[,1])))/length(na.omit(samps[,1])) # acceptance rate


[1] 0.3947
```

R code for Metropolis-Hastings - Inference



Hierarchical binomial model

Recall the hierarchical binomial model

$$Y_i \stackrel{ind}{\sim} Bin(n_i, \theta_i), \quad \theta_i \stackrel{ind}{\sim} Be(\alpha, \beta), \quad p(\alpha, \beta) \propto (\alpha + \beta)^{-5/2}$$

and after marginalizing out the θ_i

$$Y_i \stackrel{ind}{\sim} \text{Beta-binomial}(n_i, \alpha, \beta), \quad p(\alpha, \beta) \propto (\alpha + \beta)^{-5/2} \mathrm{I}(a > 0)\mathrm{I}(b > 0)$$

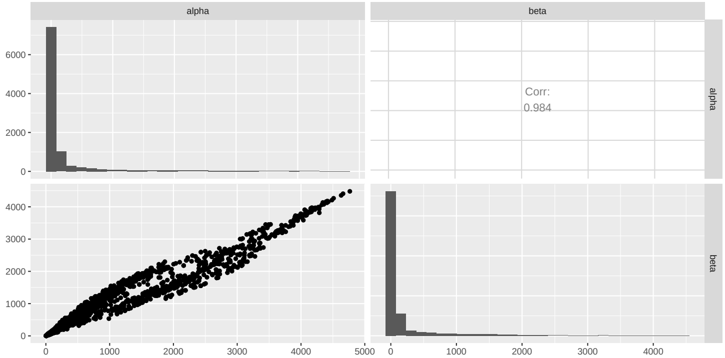
Thus the posterior is

$$p(\alpha, \beta | y) \propto \left[\prod_{i=1}^{n} \frac{B(\alpha + y_i, \beta + n_i - y_i)}{B(\alpha, \beta)} \right] (\alpha + \beta)^{-5/2} \mathrm{I}(a > 0)\mathrm{I}(b > 0)$$

where $B(\cdot)$ is the beta function.

We can perform exactly the same adapting procedure, but now using this posterior as the target distribution.

Beta-binomial hyperparameter posterior



Metropolis-Hastings summary

- The Metropolis-Hastings algorithm, samples $\theta^* \sim g(\cdot|\theta^{(t)})$ and sets $\theta^{(t+1)} = \theta^*$ with probability equal to $\min\{1, r\}$ where

$$r = \frac{q(\theta^*|y)}{q(\theta^{(t)}|y)} \frac{g(\theta^{(t)}|\theta^*)}{g(\theta^*|\theta^{(t)})}$$

  and otherwise sets $\theta^{(t+1)} = \theta^{(t)}$.
- There are two common Metropolis-Hastings proposals
  - independent proposal: $g(\theta^*|\theta^{(t)}) = g(\theta^*)$
  - random-walk proposal: $g(\theta^*|\theta^{(t)}) = g(\theta^{(t)}|\theta^*)$
- Independent proposals suffer from the same heavy-tail problems as rejection sampling proposals.
- Random-walk proposals require tuning of the random walk parameter.