

# Metropolis-Hastings algorithm

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# 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

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

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.

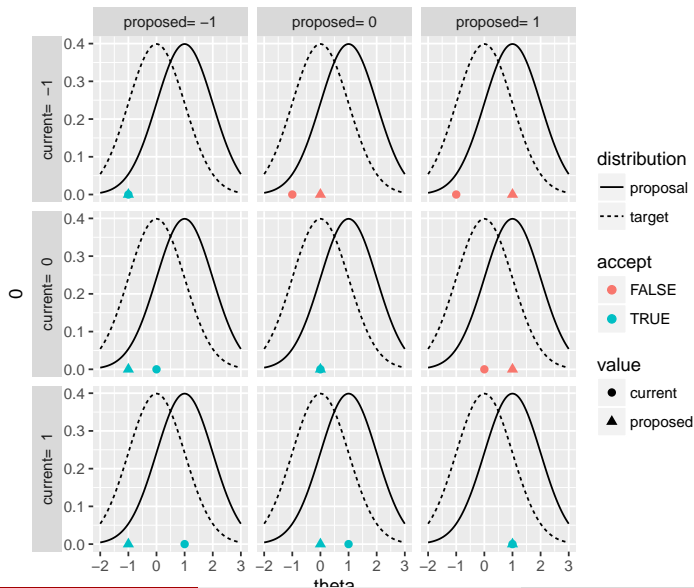
The **independence Metropolis-Hastings algorithm** performs the following

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  $\theta \sim \text{Ca}(0, 1)$  such that the posterior is

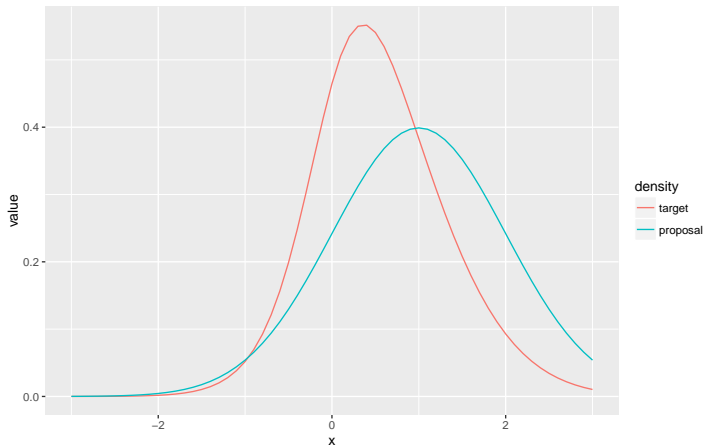
$$p(\theta|y) \propto p(y|\theta)p(\theta) \propto \frac{\exp(-(y - \theta)^2/2)}{1 + \theta^2}$$

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

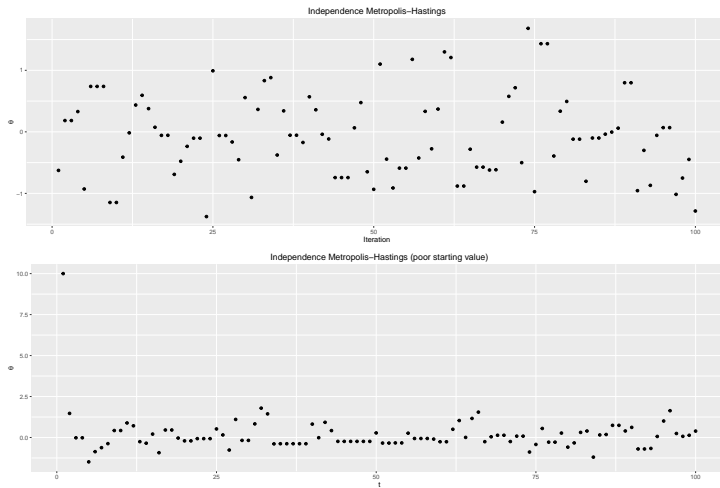
$$\begin{aligned} r &= \frac{q(\theta^*|y) \, g(\theta^{(t)})}{q(\theta^{(t)}|y) \, g(\theta^*)} \\ &= \frac{\exp(-(y - \theta^*)^2/2)/1 + (\theta^*)^2}{\exp(-(y - \theta^{(t)})^2/2)/1 + (\theta^{(t)})^2} \frac{\exp(-(\theta^{(t)} - y)^2/2)}{\exp(-(\theta^* - y)^2/2)} \\ &= \frac{1 + (\theta^{(t)})^2}{1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



# 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 since if  $\theta^{(t)}$  is

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

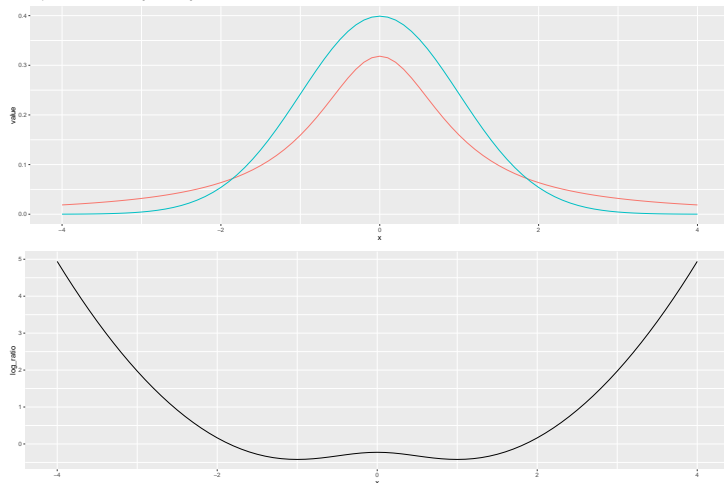
will result in

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

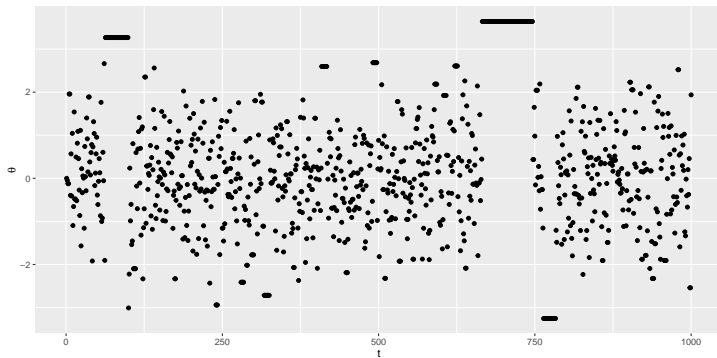
and few samples will be accepted.

# Need heavy tails - example

Suppose  $\theta|y \sim \text{Ca}(0, 1)$  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

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

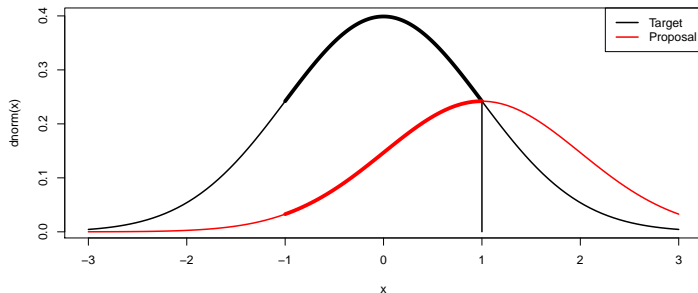
otherwise, set  $\theta^{t+1} = \theta^{(t)}$ .

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

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

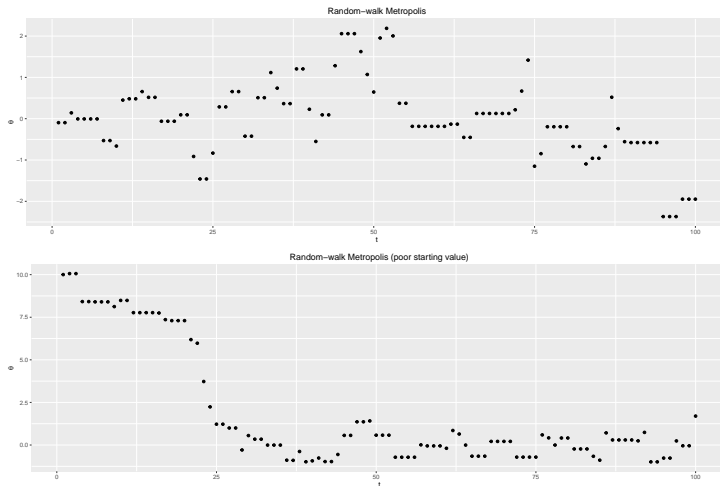
Use  $N(\theta^{(t)}, \tau^2)$  as the proposal, then the acceptance probability is the  $\min\{1, r\}$  with

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

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

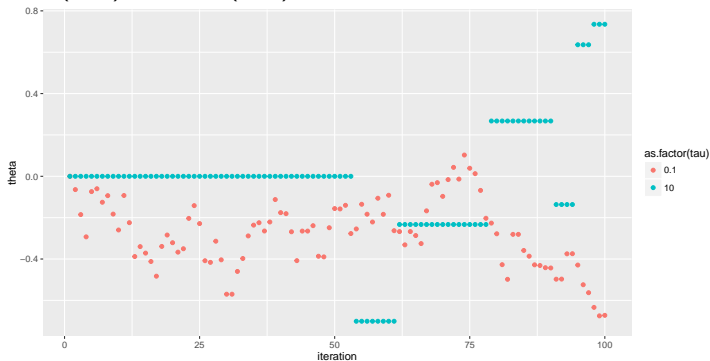
$$r = \frac{q(\theta^*|y)}{q(\theta^{(t)}|y)} \approx 0$$

so all proposed values are rejected.

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

# 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  $Y \sim \text{Bin}(n, \theta)$  and  $\theta \sim \text{Be}(1/2, 1/2)$ , thus the posterior is

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

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

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

# 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

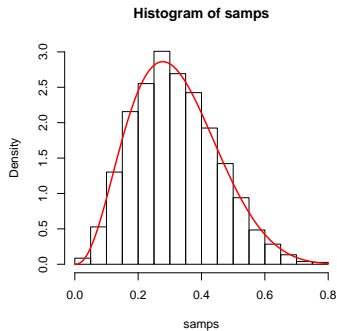
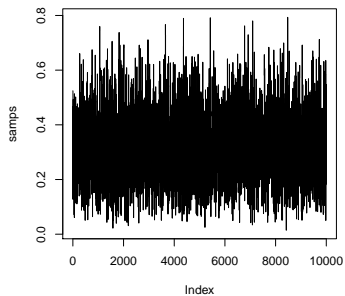
  logr = log_q(proposed)-log_q(current)
  if (log(runif(1)) < logr) current = proposed

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

[1] 0.3746

```

# Binomial



# Normal model

Assume

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

and thus

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

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

$$\begin{pmatrix} \mu^* \\ \sigma^* \end{pmatrix} \sim N \left( \begin{bmatrix} \mu^{(t)} \\ \sigma^{(t)} \end{bmatrix}, \Sigma \right)$$

where  $\Sigma$  is the tuning parameter.

## Adapting the tuning parameter

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

Proposed automatic adapting of the Metropolis-Hastings tuning parameter:

1. Start with  $\Sigma_0$ . Set  $b = 0$ .
2. Run  $M$  iterations of the MCMC using  $2.4^2 \Sigma_b/d$ .
3. Set  $\Sigma_{b+1}$  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

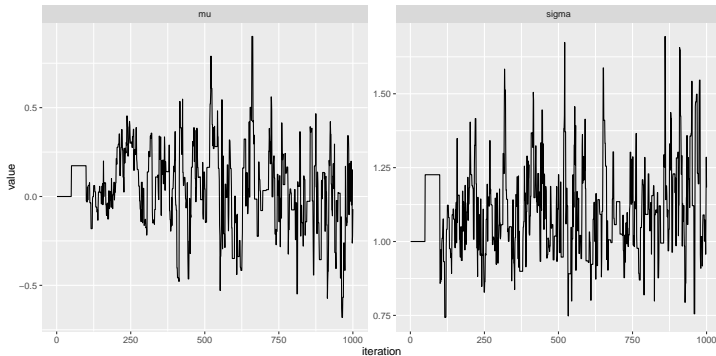
[1] 0.0300000 0.2700000 0.3566667 0.4000000 0.4240000 0.4333333 0.4200000 0.4175000 0.4166667 0.4270000

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')
```



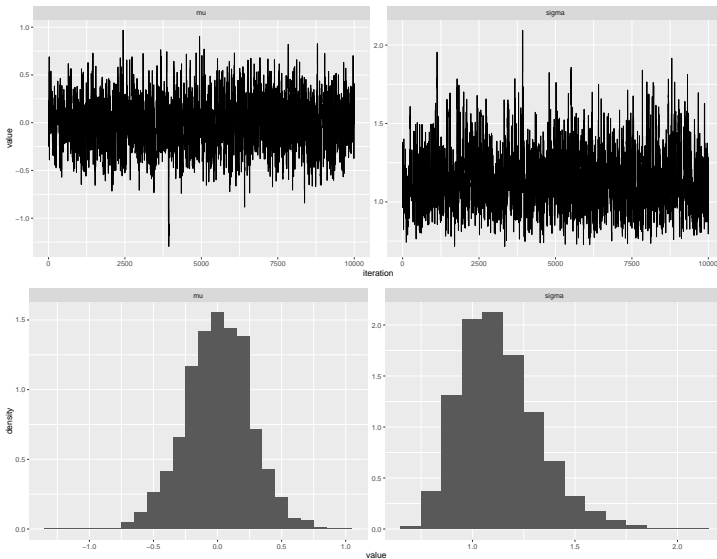
# R code for Metropolis-Hastings - Inference

```
# 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

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

and after marginalizing out the  $\theta_i$

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

Thus the posterior is

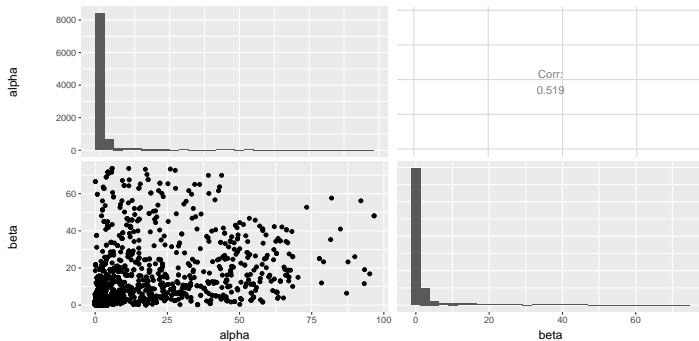
$$p(\alpha, \beta | y) \propto \left[ \prod_{i=1}^n \frac{B(\alpha + y_i, \beta + n_i - y_i)}{B(\alpha, \beta)} \right] (\alpha + \beta)^{-5/2} \text{I}(a > 0) \text{I}(b > 0)$$

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

```
Warning in file(file, "rt"): cannot open file 'Ch05a-dawkins.csv': No such file or directory
Error in file(file, "rt"): cannot open the connection
```



# 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.