

# Introduction to Bayesian Data Analysis

ZHANG Xiaowei  
HKUST

# Self-introduction (张晓炜)

- Education
  - Ph.D. in Operations Research, Stanford University, 2011
  - B.S. in Mathematics, Nankai University, 2006
- Research
  - stochastic simulation
  - data-based service engineering

# Overview

# Part 1. Fundamentals of Bayesian Inference

- What and why?
- One-parameter models
  - Binomial model
  - Poisson model
  - Exponential family and conjugate priors
- Normal model
  - Infer mean with known variance
  - Jointly infer mean and variance

## Part 2. Monte Carlo Methods

- Basic Monte Carlo
  - Monte Carlo integration
  - Random variable generation
- Markov chain Monte Carlo
  - Slice sampler
  - Metropolis-Hastings algorithms
  - Gibbs sampler

# 1. What and Why?

# Probability

- I have 50% probability of getting a head when flipping a coin
- An Olympic shooter has 95% probability of hitting the target
- Weather forecast indicates 80% probability of raining tomorrow
- A cancer patient was told that he had 60% chance of surviving for at least 5 years
- There are two possible ways to interpret probability
  - Frequency
  - Belief

# Frequency

- Classical.
- Example. We expect to get a head about half the time if we flip a coin many many times
- However, repeated experiments are not possible in many situations
  - What is the probability that another terrorist attack of the “9-11” scale would happen in 10 years?

# Belief

- Quantifies a particular person's subjective opinion as to how likely an event is to occur
- Not limited to repeatable events
- Different people have different probabilities regarding the same event
  - This is part of the reason why Bayesian statistics is controversial
  - Many people insist that probability should be *objective*

- The same person's subjective probability is likely to change as more information becomes available
  - Bayes' rule stipulates how one should update his belief with new information
  - Bayesian learning is a mathematical formulation of this process

- Here are several statements about John. After reading them, what is your belief regarding whether he is a thief?
  - He was wearing a mask standing in front of a jewelry store
  - An alarm was set off at the same time
  - He was the owner of the store
    - He just return from a masquerade party
    - He didn't have the key with him

# Bayes' Rule

- There are two quantities of central interest
  - $\theta$ : a parameter that expresses the characteristics of a system
  - $Y$ : a dataset that is generated by observing the system
- Bayesian inference begins with a formulation of joint beliefs about  $\theta$  and  $Y$ 
  1. *Prior distribution*  $p(\theta)$ : describes our belief about the  $\theta$  before seeing the dataset  $Y$
  2. *Likelihood*  $p(y|\theta)$ : describes our belief about  $Y$  if we knew the value of  $\theta$ 
    - also called *sampling model*

- Once the dataset  $Y$  becomes available, the last step is to update our belief about  $\theta$
- 3. *Posterior distribution  $p(\theta|y)$ : describes our belief about  $\theta$  having observed dataset  $Y$*

$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{\int p(y|\tilde{\theta})p(\tilde{\theta}) d\tilde{\theta}}$$

- Bayes' rule does not tell us what our beliefs should be, it tells us how they should change after seeing new information*

# Why Bayes?

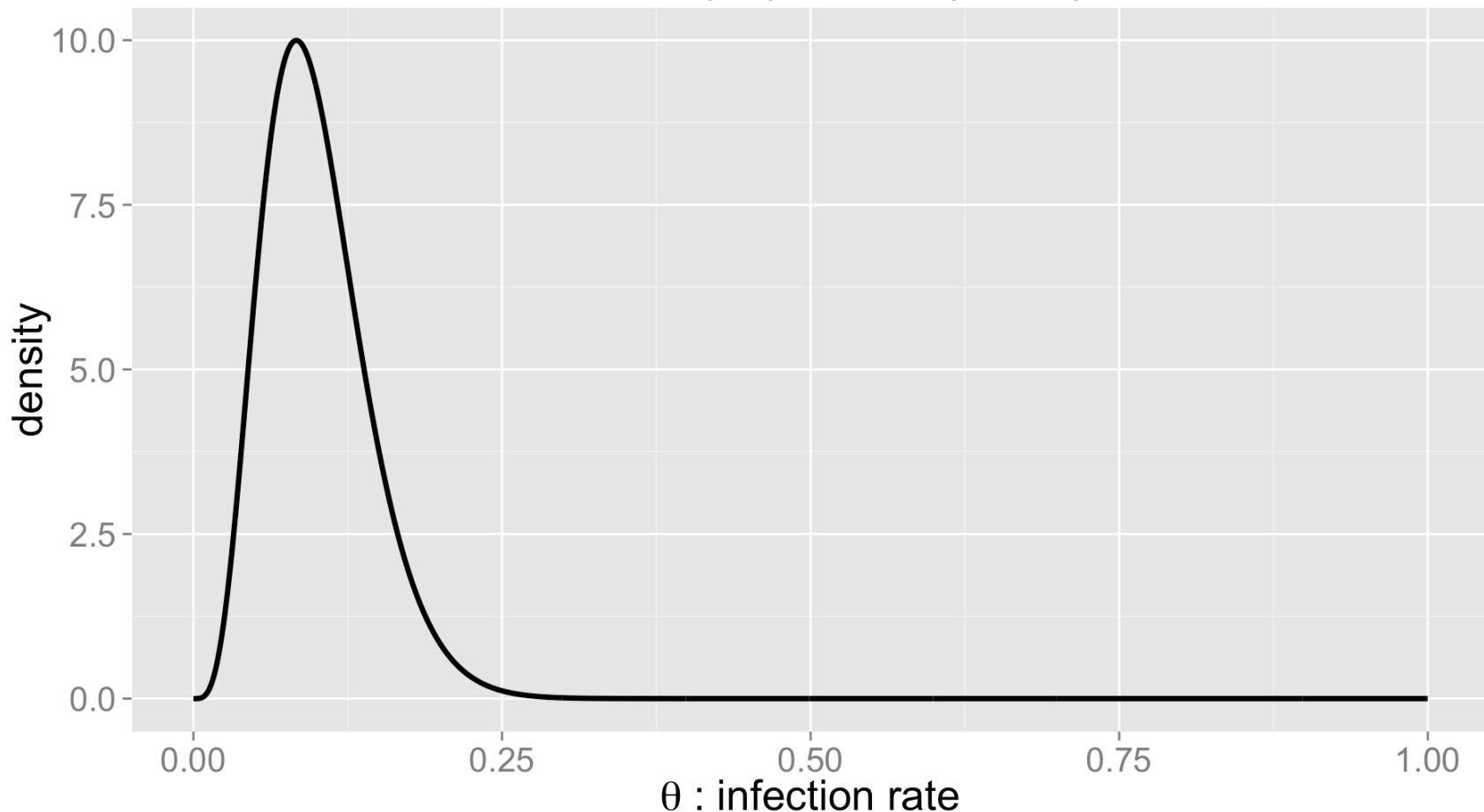
- We are interested in the prevalence of flu in a small city
- A small random sample of 20 individuals from the city will be checked
- $\theta$ : infection rate in the city
- $Y$ : total number of people in the sample who are infected

## Prior

- Studies in comparable cities indicate that the infection rate ranges from 0.05 to 0.20, with an average of 0.10
- There are infinitely many candidates and we use one that is *analytically tractable* for computational convenience
  - assume  $p(\theta)$  is beta( $a, b$ )
  - $a$  and  $b$  are called *hyperparameters*

- We select  $a = 5$  and  $b = 45$  so that
  - $E[\theta] = \frac{a}{a+b} = 0.1$
  - $\text{mode}[\theta] = \frac{a-1}{a+b-2} = 0.0833$
  - $P(\theta \in (0.05, 0.20)) = 0.8815$

Prior:  $p(\theta) = \text{beta}(5, 45)$

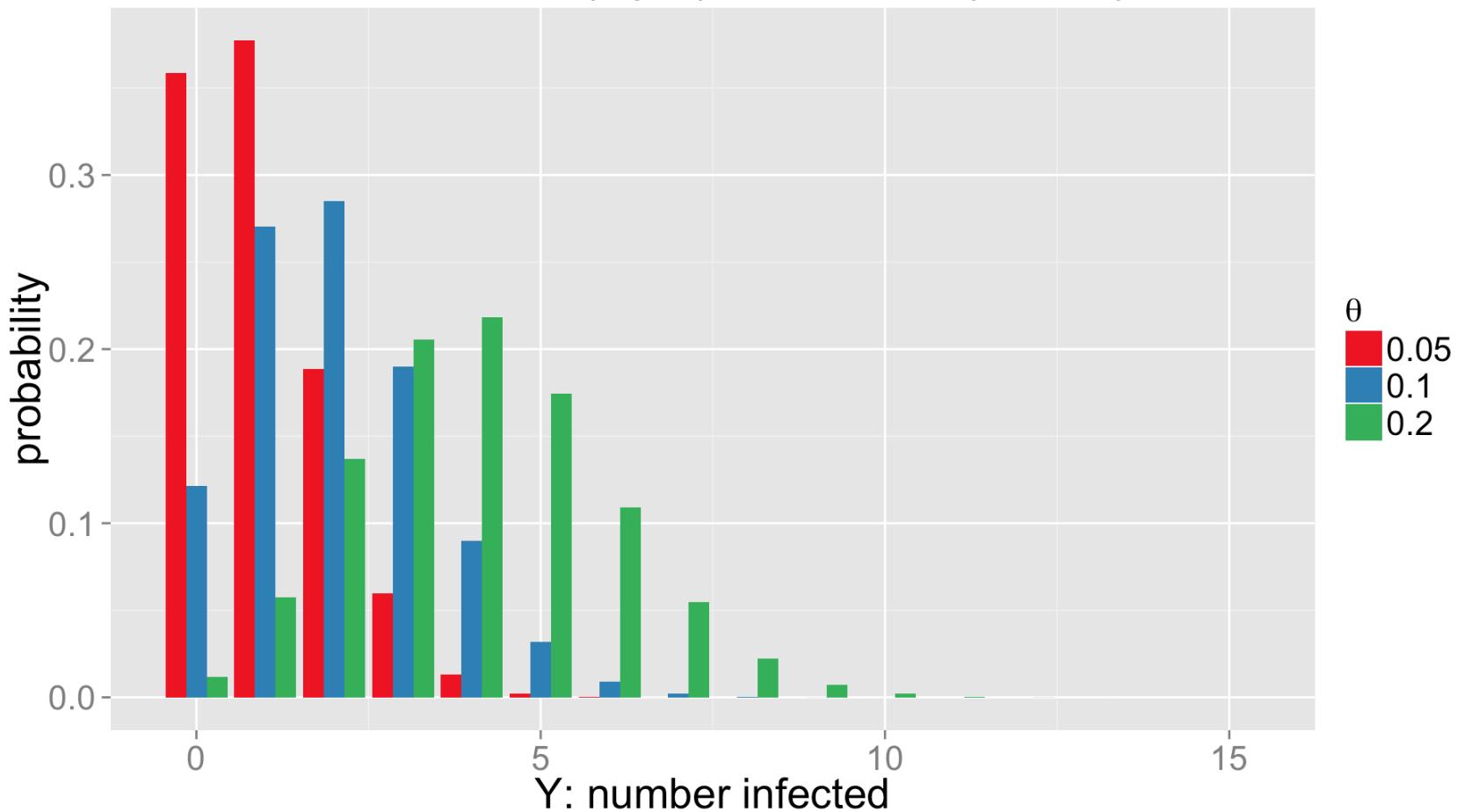


# Likelihood

- If the value of  $\theta$  were known, then  $Y$  can be modeled as a binomial distribution

$$Y|\theta \sim \text{binomial}(20, \theta)$$

Likelihood:  $p(Y|\theta) = \text{binomial}(20, \theta)$



## Posterior

- We will see that if  $\theta \sim \text{beta}(a, b)$  and  $Y|\theta \sim \text{binomial}(n, \theta)$ , then the posterior distribution is beta too!

$$\theta|Y \sim \text{beta}(a + Y, b + n - Y)$$

- Suppose half of the sampled individuals are infected, i.e.

$$Y = 10$$

- $E[|Y=10] = \$0.2143$

- $\$[|Y=10] = \$0.2059$

- 95% confidence interval is  $(0.1212, 0.3094)$ , i.e.

$$P(\theta \in (0.1212, 0.3094) | Y = 10) = 95\%$$

## Comparison to Frequentist Approach

- No prior information is needed
- Point estimate:  $\hat{\theta} = \frac{Y}{n}$
- 95% confidence interval is  $\hat{\theta} \pm 1.96 \sqrt{\frac{\hat{\theta}(1-\hat{\theta})}{n}}$ 
  - With  $Y = 10$ , it is  $(0.2809, 0.7191)$ , much wider than the Bayesian counterpart
  - *Prior information helps reduce uncertainty!*

## 2. One-parameter Models

# Binomial Model

- $Y$  has binomial distribution with parameter  $n$  and  $\theta$ 
  - $n$  is known,  $\theta$  is unknown
  - $Y$  is number of “successes” in  $n$  independent trials
    - sum of  $n$  i.i.d. Bernoulli random variables
  - Each trial has  $\theta$  probability of success
- Likelihood:  $Y|\theta \sim \text{binomial}(n, \theta)$

$$p(Y|\theta) = \binom{n}{Y} \theta^Y (1 - \theta)^{n-Y}$$

## Uniform Prior

- Each value has equal possibility:  $\theta \sim \text{uniform}[0, 1]$   
$$p(\theta) = 1$$

■ A *noninformative* prior

- Bayes' rule asserts:

$$p(\theta|Y) = \frac{p(Y|\theta)p(\theta)}{p(Y)} = \frac{p(Y|\theta)}{p(Y)} \propto p(Y|\theta)$$

- $\propto$  means “is proportional to”
  - $p(\theta|Y)$  is proportional to  $p(Y|\theta)$  as a function of  $\theta$
  - because  $p(Y)$  does not depend on  $\theta$

- Further, we can see that

$$p(\theta|Y) \propto \theta^Y (1-\theta)^{n-Y}$$

- So if we assume  $p(\theta|Y) = C\theta^Y (1-\theta)^{n-Y}$  for some constant  $C > 0$ , then

$$C^{-1} = \int_0^1 \theta^Y (1-\theta)^{n-Y} d\theta = B(Y+1, n-Y+1),$$

where  $B$  is the beta function, because  $\int_0^1 p(\theta|Y) d\theta = 1$

- So

$$p(\theta|Y) = \frac{\theta^Y (1-\theta)^{n-Y}}{B(Y+1, n-Y+1)},$$

i.e.  $\theta|Y \sim \text{beta}(Y+1, n-Y+1)$

## Beta Prior

- $\theta \sim \text{beta}(a, b)$

$$p(\theta) = \frac{\theta^{a-1}(1-\theta)^{b-1}}{B(a, b)}$$

- Uniform distribution is a special case of beta distribution
  - uniform[0,1] = beta(1,1)
- Applying Bayes' rule

$$p(\theta|Y) \propto p(Y|\theta)p(\theta)$$

$$= \binom{n}{Y} \theta^Y (1-\theta)^{n-Y} \times \frac{\theta^{a-1}(1-\theta)^{b-1}}{B(a, b)}$$

so  $p(\theta|Y) = C\theta^{a+Y-1}(1-\theta)^{b+n-Y-1}$  for some positive constant  $C$ , where

$$\begin{aligned}
C^{-1} &= \int_0^1 \theta^{a+Y-1} (1-\theta)^{b+n-Y-1} d\theta \\
&= B(a+Y, b+n-Y)
\end{aligned}$$

- So the posterior distribution is  $\text{beta}(a+Y, b+n-Y)$ , i.e.

$$p(\theta|Y) = \frac{\theta^{a+Y-1} (1-\theta)^{b+n-Y-1}}{B(a+Y, b+n-Y)}$$

# Conjugacy

- A class  $\mathcal{P}$  of prior distributions for  $\theta$  is called *conjugate* for a sampling model  $p(y|\theta)$  if

$$p(\theta) \in \mathcal{P} \Rightarrow p(\theta|y) \in \mathcal{P}$$

- Conjugate priors make posterior calculations easy
- but might not actually represent our prior information
- Beta prior is conjugate for the binomial sampling model

# Combining Information

- $\theta|Y \sim \text{beta}(a + Y, b + n - Y)$

$$\begin{aligned} E[\theta|Y = y] &= \frac{a + y}{a + b + n} \\ &= \frac{n}{a + b + n} \cdot \hat{\theta} + \frac{a + b}{a + b + n} \cdot \theta_0 \end{aligned}$$

- $\hat{\theta} = \frac{y}{n}$  is the frequentist estimate of  $\theta$
- $\theta_0 = \frac{a}{a+b}$  is the prior expectation of  $\theta$

1. The posterior expectation is the *weighted average* of  $\hat{\theta}$  and  $\theta_0$
2. The weight of  $\theta_0$  vanishes as  $n \rightarrow \infty$ 
  - The impact of prior information gradually fades away when the dataset is sufficiently large

## Prediction

- Let  $\tilde{Y}$  be an additional outcome from the same population
- *Predictive distribution:*  $p(\tilde{Y}|Y)$

$$P(\tilde{Y} = k|Y)$$

$$= \int P(\tilde{Y} = k|\theta, Y)p(\theta|Y) d\theta$$

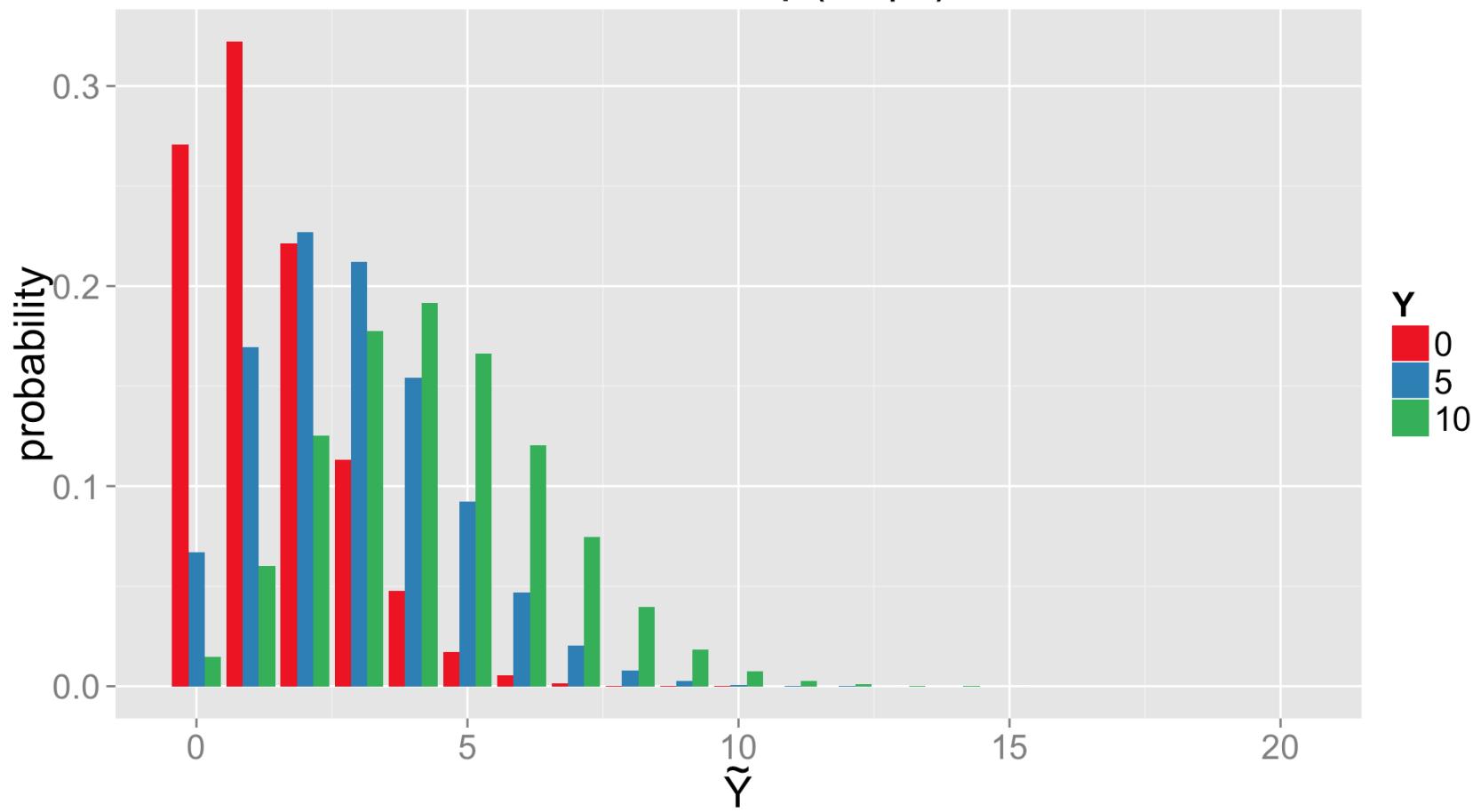
$$= \int_0^1 \binom{n}{k} \theta^k (1-\theta)^{n-k} \cdot \frac{\theta^{a+Y-1} (1-\theta)^{b+n-Y-1}}{B(a+Y, b+n-Y)} d\theta$$

$$= \binom{n}{k} \frac{B(a+Y+k, b+2n-Y-k)}{B(a+Y, b+n-Y)}$$

```
pred_dist <- function(k, Y, a, b, n) {
  choose(n, k) * beta(a + Y + k, b + 2 * n - Y - k)/beta(a + Y, b + n - Y)
}
a <- 5
b <- 45
n <- 20
Y <- 10
pred_dist(seq(0, n), Y, a, b, n)

## [1] 1.485e-02 6.022e-02 1.254e-01 1.776e-01 1.914e-01 1.662e-01 1.205e-01
## [8] 7.440e-02 3.970e-02 1.845e-02 7.492e-03 2.661e-03 8.235e-04 2.207e-04
## [15] 5.065e-05 9.792e-06 1.556e-06 1.957e-07 1.831e-08 1.136e-09 3.511e-11
```

## Predictive: $p(\tilde{Y} | Y)$



- The predictive distribution does not depend on any unknown quantities
  - It is calculated by “integrating out” the uncertainty about  $\theta$
- $\tilde{Y}$  is not independent of  $Y$ 
  - $Y$  gives information about  $\theta$ , which in turn gives information about  $\tilde{Y}$

# Confidence Regions

- Regions of the parameter space that contains the true value of the parameter with high probability
  - After observing the data  $Y = y$ , construct an interval  $[l(y), u(y)]$  such that  $P(l(y) < \theta < u(y))$  is large

- *Bayesian coverage*: an interval  $[l(y), u(y)]$  has  $100(1 - \alpha)\%$  Bayesian coverage for  $\theta$  if, *after* the data are observed,  

$$P(l(y) < \theta < u(y)|Y = y) = 1 - \alpha$$
- *Frequentist coverage*: a random interval  $[l(Y), u(Y)]$  has  $100(1 - \alpha)\%$  frequentist coverage for  $\theta$  if, *before* the data are observed,  

$$P(l(Y) < \theta < u(Y)|\theta) = 1 - \alpha$$
- In a sense, the frequentist and Bayesian notions of coverage describe pre- and post-experimental coverage, respectively.

# Quantile-based Intervals

- Remove both tails of  $\alpha/2$  probability
- Use  $[\theta_{\alpha/2}, \theta_{1-\alpha/2}]$ , where  $\theta_{\alpha/2}$  and  $\theta_{1-\alpha/2}$  are posterior quantiles

$$P(\theta < \theta_{\alpha/2} | Y = y) = P(\theta > \theta_{1-\alpha/2} | Y = y) = \alpha/2$$

- Easy to implement

```
a <- 5; b <- 45; n <- 20; Y <- 10;  
qbeta(c(0.025, 0.975), a + Y, b + n - Y)  
  
## [1] 0.1271 0.3169
```

## Highest Posterior Density Region

- If the posterior distribution is not *symmetric*, a quantile-based interval excludes some points that have higher density than some points inside the interval
- *HPD region*: a subset of the parameter space  $s(y)$  such that
  1.  $P(\theta \in s(y) | Y = y) = 1 - \alpha$
  2.  $p(\theta_1 | Y = y) > p(\theta_2 | Y = y)$  for  $\theta_1 \in s(y)$  and  $\theta_2 \notin s(y)$
- May not be an interval if the posterior density is *multimodal*, i.e. has multiple peaks

- Harder to implement: usually apply simulation to approximate

```
a <- 5; b <- 45; n <- 20; Y <- 10;  
require(hdrcde)  
as.vector(hdr(rbeta(1e5, a + Y, b + n - Y), prob=95)$hdr)
```

```
## [1] 0.1213 0.3098
```

# Poisson Model

- Usually models the number of events occurring in a fixed time period
- Likelihood:  $Y|\theta \sim \text{Poisson}(\theta)$

$$p(Y|\theta) = \frac{\theta^Y e^{-\theta}}{Y!}$$

- $E[Y|\theta] = \text{var}(Y|\theta) = \theta$

## Gamma Prior

- $\theta \sim \text{Gamma}(a, b)$ 
  - $a$  is the shape parameter and  $b$  is the rate parameter

$$p(\theta) = \frac{b^a}{\Gamma(a)} \theta^{a-1} e^{-b\theta}$$

- $E[\theta] = \frac{a}{b}$

## Posterior

- By Bayes' rule,

$$p(\theta|Y) \propto p(Y|\theta)p(\theta) = \frac{\theta^Y e^{-\theta}}{Y!} \times \frac{b^a}{\Gamma(a)} \theta^{a-1} e^{-b\theta}$$

- So  $p(\theta|Y) = C\theta^{a+Y-1}e^{-(b+1)\theta}$ , where

$$C^{-1} = \int_0^\infty \theta^{a+Y-1} e^{-(b+1)\theta} d\theta = \frac{\Gamma(a+Y)}{(b+1)^{a+Y}}$$

- So

$$p(\theta|Y) = \frac{(b+1)^{a+Y}}{\Gamma(a+Y)} \theta^{a+Y-1} e^{-(b+1)\theta},$$

i.e.  $\theta|Y \sim \text{Gamma}(a+Y, b+1)$

- Gamma prior is conjugate for the Poisson sampling model

# Combining Information

- Suppose  $Y_1, \dots, Y_n$  are i.i.d. Poisson

- Then  $\theta|Y_1, \dots, Y_n \sim \text{Gamma}(a + \sum_{i=1}^n Y_i, b + n)$

$$\begin{aligned} E[\theta|Y_1, \dots, Y_n] &= \frac{a + \sum_{i=1}^n Y_i}{b + n} \\ &= \frac{n}{b + n} \cdot \hat{\theta} + \frac{b}{b + n} \cdot \theta_0 \end{aligned}$$

- $\hat{\theta} = \frac{\sum_{i=1}^n Y_i}{n}$  is the frequentist estimate of  $\theta$

- $\theta_0 = \frac{a}{b}$  is the prior expectation of  $\theta$

1. The posterior expectation is the weighted average of  $\hat{\theta}$  and  $\theta_0$
2. The weight of  $\theta_0$  vanishes as  $n \rightarrow \infty$ 
  - The impact of prior information gradually fades away when the dataset is sufficiently large

## Prediction

- The predictive distribution of  $\tilde{Y}$ , an additional outcome from the same population, given the observation  $Y$

$$\begin{aligned} & P(\tilde{Y} = k|Y) \\ &= \int_0^\infty P(\tilde{Y} = k|\theta)p(\theta|Y) d\theta \\ &= \int_0^\infty \frac{\theta^k e^{-\theta}}{k!} \cdot \frac{(b+1)^{a+Y}\theta^{a+Y-1}e^{-(b+1)\theta}}{\Gamma(a+Y)} d\theta \\ &= \frac{\Gamma(a+Y+k)}{\Gamma(k+1)\Gamma(a+Y)} \left( \frac{b+1}{b+2} \right)^{a+Y} \left( \frac{1}{b+2} \right)^k \end{aligned}$$

- So  $\tilde{Y}|Y$  has a negative binomial distribution with “number of failures”  $a + Y$  and “success probability”  $\frac{1}{b+2}$

```
a <- 2; b <- 1; Y <- 5;
dnbinom(seq(0, 10), a + Y, 1 / (b + 2))

## [1] 0.0004572 0.0021338 0.0056902 0.0113804 0.0189673 0.0278187 0.0370916
## [8] 0.0459229 0.0535768 0.0595297 0.0634984
```

# Exponential Families and Conjugate Priors

- Both binomial and Poisson models belong to one-parameter *exponential family models*, whose densities are of the form

$$p(y|\theta) = a(y)e^{\phi(\theta)t(y)+b(\theta)}$$

- Binomial model

$$\phi(\theta) = \log\left(\frac{\theta}{1-\theta}\right), t(y) = y, b(\theta) = n \log(1 - \theta), a(y) = \binom{n}{y}$$

- Poisson model

$$\phi(\theta) = \log \theta, t(y) = y, b(\theta) = -\log(\theta), a(y) = 1$$

- Exponential model

$$\phi(\theta) = -\theta, t(y) = y, b(\theta) = \log(\theta), a(y) = 1$$

- Normal model (with  $\sigma^2$  known)

$$\phi(\theta) = \frac{\theta}{\sigma^2}, t(y) = y, b(\theta) = -\frac{\theta^2}{2\sigma^2}, a(y) = \exp\left(-\frac{y^2}{2\sigma^2}\right)$$

- Choose a prior of the form  $p(\theta) = k(\alpha, \beta)e^{\alpha\phi(\theta)+\beta b(\theta)}$
- Then the posterior is

$$p(\theta|Y) \propto e^{(\alpha+t(Y))\phi(\theta)+(\beta+1)b(\theta)}$$

- So the prior is conjugate for the exponential family model
- In general, the posterior conditional on the i.i.d. data

$Y_1, \dots, Y_n$  is

$$p(\theta|Y_1, \dots, Y_n) \propto e^{(\alpha+\sum_{i=1}^n t(Y_i))\phi(\theta)+(\beta+n)b(\theta)}$$

### 3. Normal Model

# Normal Model

- Normal distribution is probably the most useful probability model in statistics
  - supported by central limit theorem
  - two parameters, mean  $\mu$  and variance  $\sigma^2$ , are often of primary interest

$$p(y|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right), \quad -\infty < y < \infty$$

- the distribution is symmetric about  $\theta$ , and the mode, median and mean are all equal to  $\theta$
- about 95% of the population lies within two standard deviations of the mean (more precisely, 1.96 standard deviations)

# Inference on Mean with Known Variance

- Choose a normal prior on the mean, i.e.  $\mu \sim \text{normal}(\mu_0, \tau_0)$

$$p(\mu|Y, \sigma^2) = \frac{p(\mu|\sigma^2)p(Y|\mu, \sigma^2)}{p(Y|\sigma^2)} \propto p(\mu|\sigma^2)p(Y|\mu, \sigma^2)$$
$$\propto \exp\left(-\frac{(\mu-\mu_0)^2}{2\tau_0}\right) \exp\left(-\frac{(Y-\mu)^2}{2\sigma^2}\right)$$

- The exponent is quadratic in  $\mu$  so  $p(\mu|Y, \sigma^2)$  is normal with mean

$$\frac{\frac{1}{\tau_0^2} \mu_0 + \frac{1}{\sigma^2} Y}{\frac{1}{\tau_0^2} + \frac{1}{\sigma^2}}$$

and variance

$$\frac{1}{\frac{1}{\tau_0^2} + \frac{1}{\sigma^2}}$$

- In general, given i.i.d. normal data  $Y_1, \dots, Y_n$ , if we select a normal prior on  $\mu$ , then  $p(\mu|Y_1, \dots, Y_n, \sigma^2)$  is normal with mean  $\mu_n$  and variance  $\tau_n^2$ , where

$$\mu_n = \frac{\frac{1}{\tau_0^2} \mu_0 + \frac{n}{\sigma^2} \bar{Y}}{\frac{1}{\tau_0^2} + \frac{n}{\sigma^2}} \quad \text{and} \quad \tau_n^2 = \frac{1}{\frac{1}{\tau_0^2} + \frac{n}{\sigma^2}}$$

- Inverse variance is often called *precision* and it quantifies the information

$$\frac{1}{\tau_n^2} = \frac{1}{\tau_0^2} + \frac{n}{\sigma^2}$$

- Posterior info = prior info + data info
- Precision is increasing in  $n$
- Posterior mean is a weighted average of the prior mean and the sample mean

$$\mu_n = \frac{\tau_0^{-2}}{\tau_0^{-2} + n\sigma^{-2}} \mu_0 + \frac{n\sigma^{-2}}{\tau_0^{-2} + n\sigma^{-2}} \bar{Y}$$

## Example

- The revenue of a Taobao shop in the past 9 months is as follows (unit: million RMB) and we hope to make inference on the mean monthly revenue.

```
## [1] 1.82 2.30 1.64 1.52 1.72 1.36 1.74 2.08 1.97
```

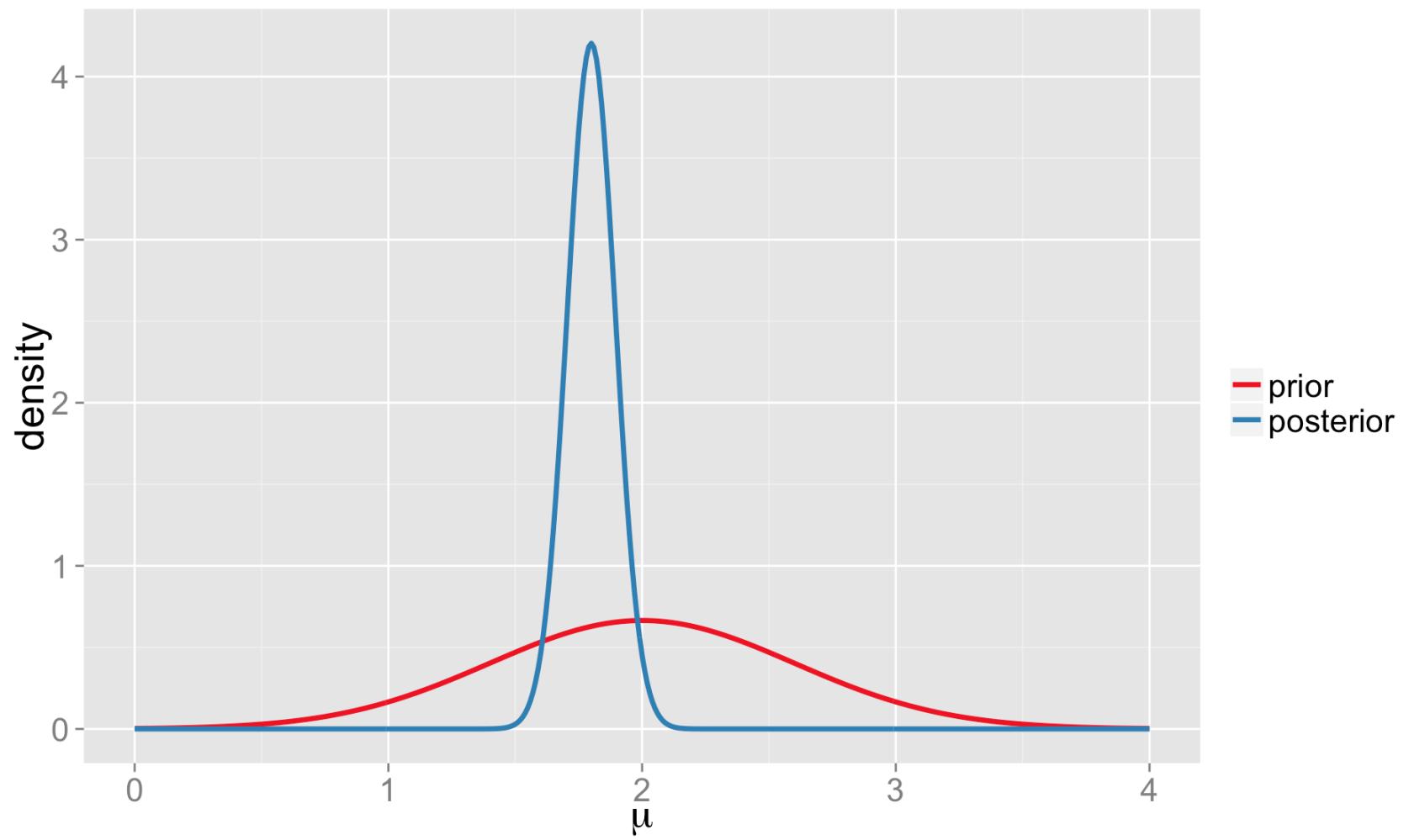
- We know the average monthly revenue in million RMB in 2012 is about 2 and its s.d. is about 0.6
  - Choose prior on  $\mu$  as  $\text{normal}(2, 0.6^2)$
- We use the sample variance as  $\sigma^2$

```

revenue <- c(1.82, 2.3, 1.64, 1.52, 1.72, 1.36, 1.74, 2.08, 1.97)
n <- length(revenue)
Y_bar <- mean(revenue)
s2 <- var(revenue)
mu_0 <- 2
tau_0 <- 0.6
a <- 1/tau_0^2 + n/s2
b <- mu_0/tau_0^2 + n/s2 * Y_bar
tau_n <- sqrt(1/a)
mu_n <- b/a

```

- So the posterior distribution of the average monthly revenue is normal with mean 1.7996 and s.d. 0.0949
  - Its prior is normal with mean 2 and s.d. 0.6
  - Sample mean is 1.7944 and sample s.d. is 0.2883
- Remark: posterior s.d. is smaller than both prior s.d. and sample s.d.



# Joint Inference on Mean and Variance

- In the previous example, we assumed  $\sigma^2$  is known and use the sample variance for its value
  - Due to the small sample size, the sample variance has a fairly large uncertainty in itself which we have ignored
- Hence, we need to infer  $\mu$  and  $\sigma^2$  at the same time and find a joint prior on  $(\mu, \sigma^2)$

$$p(\mu, \sigma^2 | Y_1, \dots, Y_n) \propto p(Y_1, \dots, Y_n | \mu, \sigma^2) p(\mu, \sigma^2)$$

- In choosing the joint prior  $p(\mu, \sigma^2)$ , note that
$$p(\mu, \sigma^2) = p(\mu|\sigma^2)p(\sigma^2)$$
- We have seen that if  $\sigma^2$  were known, then a conjugate prior on  $\mu$  is normal so we set  $p(\mu|\sigma^2)$  as normal
- We need a distribution that has support on  $(0, \infty)$  for  $\sigma^2$  and it turns out Gamma distribution is a crucial element

- The joint prior is chosen as follows

$$\theta|\sigma^2 \sim \text{normal}\left(\mu_0, \frac{\sigma^2}{\kappa_0}\right)$$

$$\sigma^{-2} \sim \text{gamma}\left(\frac{\nu_0}{2}, \frac{\nu_0\sigma_0}{2}\right)$$

- $\mu_0$  and  $\kappa_0$  can be interpreted as the mean and sample size from a set of prior observations

- Then using Bayes' rule, we can show that (details are left for exercise)

$$\{\mu|Y_1, \dots, Y_n, \sigma^2\} \sim \text{normal}(\mu_n, \sigma^2/\kappa_n),$$

where

$$\kappa_n = \kappa_0 + n \quad \text{and} \quad \mu_n = \frac{\kappa_0 \mu_0 + n \bar{Y}}{\kappa_n},$$

and

$$\{\sigma^{-2}|Y_1, \dots, Y_n\} \sim \text{gamma}(\nu_n/2, \nu_n \sigma_n^2/2),$$

where

$$\nu_n = \nu_0 + n$$

$$\sigma_n^2 = \frac{1}{\nu_n} [\nu_0 \sigma_0^2 + (n - 1)s^2 + \frac{\kappa_0 n}{\kappa_n} (\bar{Y} - \mu_0)^2]$$

and  $s^2$  is the sample variance of  $Y_1, \dots, Y_n$

- $\nu_0 \sigma_0^2$  and  $\nu_n \sigma_n^2$  can be interpreted as prior and posterior “sum of squared observations from the sample mean”

## Back to Previous Example

- Assume both  $\mu$  and  $\sigma^2$  are unknown
- We know the average monthly revenue in million RMB in 2012 is about 2 and its s.d. is about 0.6
  - choose prior parameters  $\mu_0 = 2, \sigma_0 = 0.6, \kappa_0 = 12$  and  $\nu_0 = 12$

```
mu_0 <- 2
sigma_0 <- 0.6
kappa_0 <- 12
nu_0 <- 12
n <- length(revenue)
Y_bar <- mean(revenue)
s2 <- var(revenue)
kappa_n <- kappa_0 + n
mu_n <- (kappa_0 * mu_0 + n * Y_bar)/kappa_n
nu_n <- nu_0 + n
sigma_n <- sqrt((nu_0 * sigma_0^2 + (n - 1) * s2 + kappa_0 * n/kappa_n * (Y_bar -
mu_0)^2)/nu_n)
```

- The posterior parameters are  $\mu_n = 1.9119$ ,  $\kappa_n = 21$ ,  $\nu_n = 21$ , and  $\sigma_n^2 = 0.2477$ .
- The posterior joint distribution of  $(\mu, \sigma^2)$  is determined by  
 $\{\mu|Y_1, \dots, Y_n, \sigma^2\} \sim \text{normal}(1.9119, \sigma^2/21)$ ,  
 $\{\sigma^{-2}|Y_1, \dots, Y_n\} \sim \text{gamma}(10.5, 2.6012)$ ,

- It can be shown that  $\frac{\mu - \mu_n}{\sigma_n / \sqrt{\kappa_n}}$  has a  $t$ -distribution with  $\nu_n$  degrees of freedom
  - This gives the *marginal* posterior distribution of  $\mu$ , i.e.  
 $p(\mu|Y_1, \dots, Y_n)$
- As expected, the uncertainty about the posterior distribution of  $\mu$  is larger when assuming  $\sigma^2$  is unknown

# Usage of Conjugate Priors is Limited

- Only exist for simple models/distributions
- Only for *computational* reasons
  - Keep distribution family fixed and update hyperparameters only
- Restricts our modeling of prior information
  - Implies a *subjective* manipulation of the prior information
  - E.g., why is the prior of a binomial distribution necessarily beta distribution?

# How do We Deal with Non-conjugate Priors?

- Monte Carlo Simulation!

# 4. Basic Monte Carlo

# Introduction

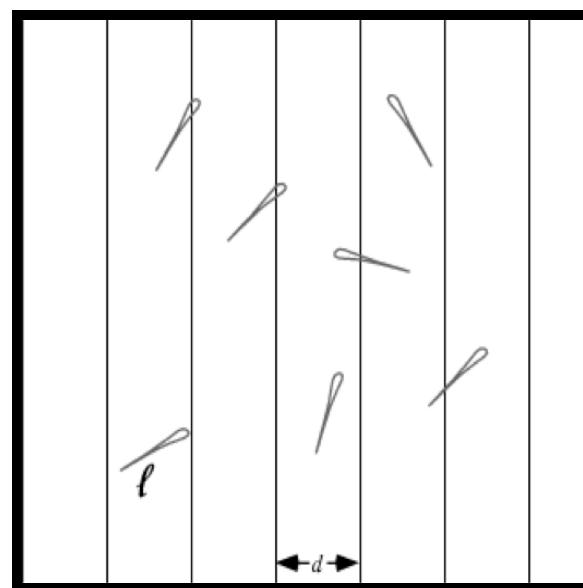
- Monte Carlo methods are a broad class of computational algorithms that rely on repeated random sampling to obtain numerical results
- One runs simulations many times to obtain the information of an unknown probabilistic entity
- Modern version of MC was invented by Stanislaw Ulam in late 1940s, while he was working on nuclear weapons projects at the Los Alamos National Laboratory

- “Monte Carlo” was named after the Monte Carlo Casino in Monte Carlo, Monaco

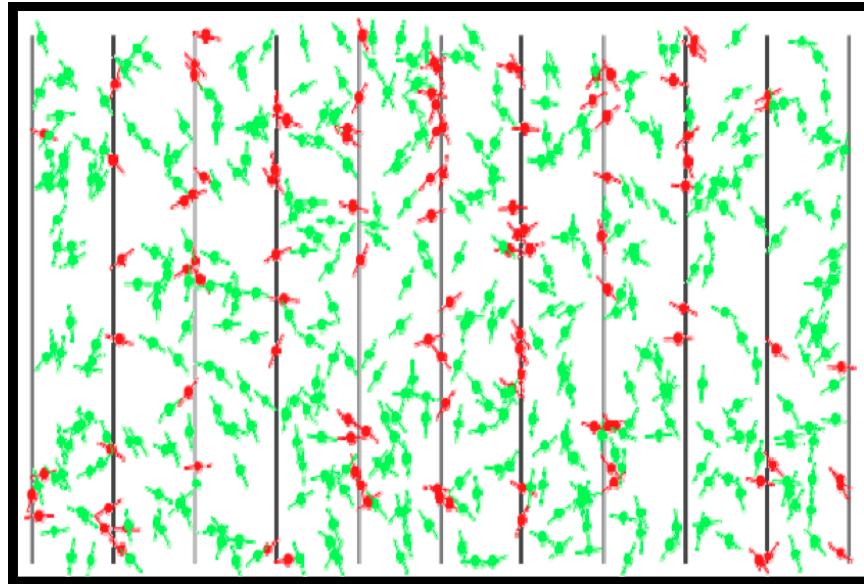


# Buffon's Needle

- The French naturalist Buffon in 1733 stated a problem: find the probability that a needle of length  $l$  will land on a line, given a floor with equally spaced parallel lines a distance  $d$  apart
  - Answer:  $p = \frac{2l}{\pi d}$  when  $d \geq l$



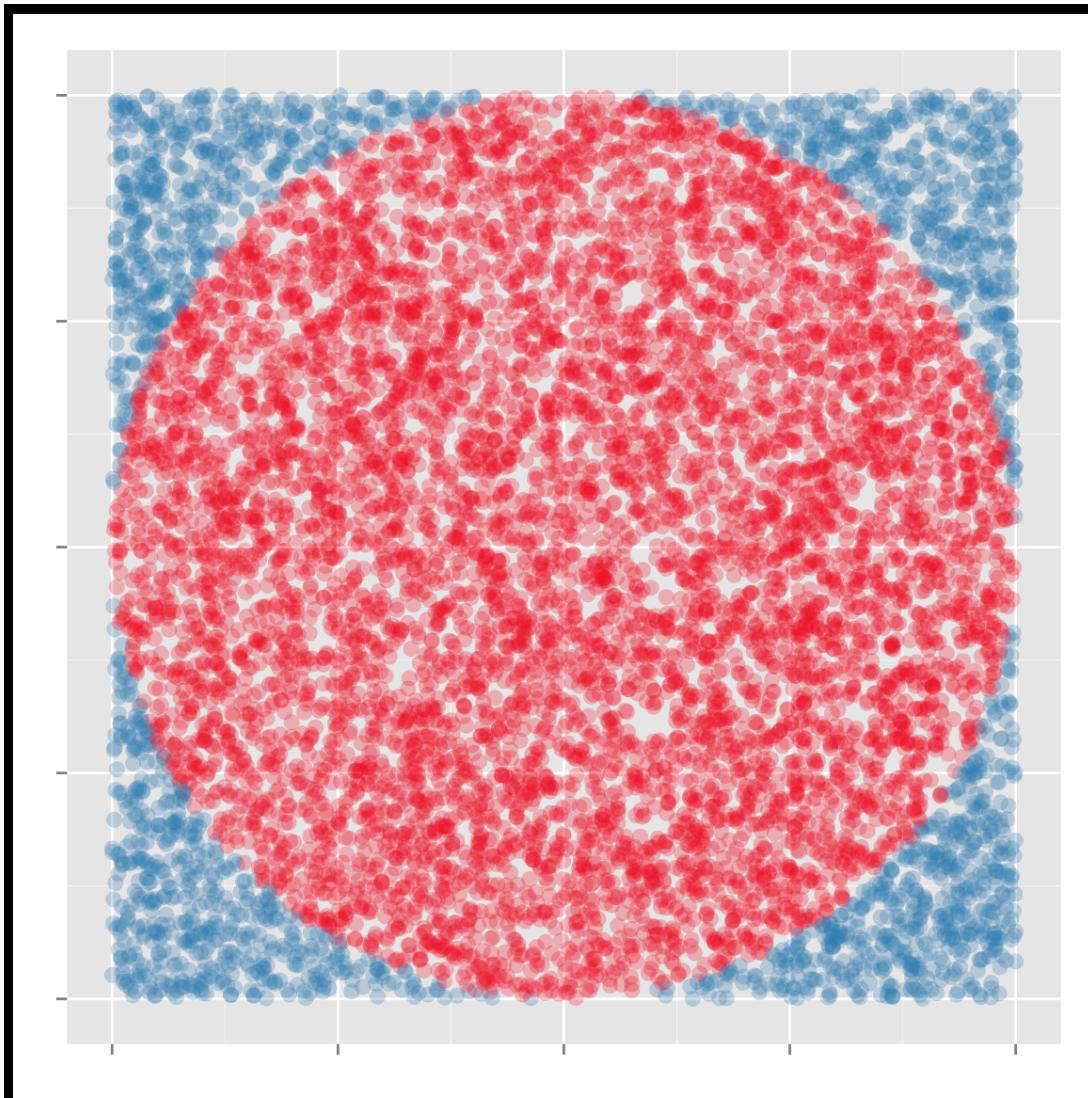
- We then can use this experiment to estimate the probability  $p$  and then the value of  $\pi$



Result of 500 random tosses of a needle with  $d = 3$  and  $l = 1$ .  
There are 107 needles cross a line, giving  $\pi \approx 3.116$ .

# Calculating $\pi$

- MC is most commonly used to evaluate integrals (including probabilities)



# Monte Carlo Integration

- Let  $X$  be a random variable with density  $f(x)$  and we are interested in computing

$$\mathbb{E}[h(X)] = \int h(x)f(x) dx$$

- MC generates a sample  $X_1, \dots, X_n$  from the density  $f$  and approximates the integral with

$$\bar{h}_n = \frac{1}{n} \sum_{j=1}^n h(X_j)$$

- Convergence (Strong Law of Large Numbers)**

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{j=1}^n h(X_j) = \mathbb{E}[h(X)]$$

## Example

- Compute  $\int_0^1 [x^2 + 4x \sin(x)] dx$ 
  - Exact value is  $\frac{1}{3} + 4[\sin(1) - \cos(1)] = 1.538$
- Write the integral as  $\mathbb{E}[X^2 + 4X \sin(X)]$  where  $X \sim \text{Uniform}(0, 1)$

```
N <- 10^4  
X <- runif(N)  
mean(X^2 + 4 * X * sin(X))  
  
## [1] 1.537
```

## Errors in MC

- Clearly, the estimation error decreases as the number of replications  $n$  increases
- But can we quantify the error for a given  $n$ ?
- Back to the previous example, plot the error against  $n$

- Error is of order  $n^{-1/2}$
- Central Limit Theorem

$$\frac{\bar{h}_n - \mathbb{E}[h(X)]}{\sqrt{\text{Var}(h(X))}} \Rightarrow \mathcal{N}(0, 1)$$

- So error is roughly  $\sqrt{\frac{\text{Var}(h(X))}{n}} \cdot N(0, 1)$  when  $n$  is large
- However,  $\text{Var}(h(X))$  is usually unknown and instead we use the sample variance  $s_n^2 = \frac{1}{n^2} \sum_{j=1}^n [h(X_j) - \bar{h}_n]^2$  to approximate it

# Random Variable Generation

- Use computer to repeatedly produce samples from the target distribution so that the empirical distribution can approximate the true distribution

$$0.2\mathcal{N}(-5, 4) + 0.5\mathcal{N}(0, 1) + 0.3\mathcal{N}(3, 0.25)$$

- Statistical software packages implement only “standard” probability distributions
- We will be concerned with generating random variables from an arbitrary density
  - For example, posterior densities are usually of the form

$$p(\theta|Y) \propto p(Y|\theta)p(\theta)$$

# Pseudo-random Numbers

- Monte Carlo simulation is fundamentally based on the production of uniform random variables between 0 and 1
- Computed-generated uniform random variables are product of a *deterministic* algorithm and not truely random
  - Given the algorithm and the *seed*, all the subsequent numbers are known with certainty
  - However, without these knowledge, they do *appear* to be random and can pass various statistical tests
  - So they're called *pseudo-random* numbers

# Linear Congruential Generator

- Simple; building block of many advanced methods
- First produces a sequence of integers

$$X_{i+1} = (aX_i + c) \mod m, \quad i = 0, 1, 2, \dots$$

- Initial value  $X_0$  is called seed

- Then transform them to numbers between 0 and 1 by

$$R_i = \frac{X_i}{m}$$

- Shortcoming: period is not long enough for modern usage

- In R, `runif` generates pseudo-random numbers and `set.seed` sets random seed
  - Random seed should be manually set only for the purpose of reproducibility of the results

```
runif(5)
```

```
## [1] 0.1454 0.8607 0.7118 0.5971 0.2862
```

```
runif(5)
```

```
## [1] 0.6748 0.5171 0.6560 0.5406 0.2624
```

```
set.seed(123)
```

```
runif(5)
```

```
## [1] 0.2876 0.7883 0.4090 0.8830 0.9405
```

```
set.seed(123)
```

```
runif(5)
```

```
## [1] 0.2876 0.7883 0.4090 0.8830 0.9405
```

# Inverse Transform Method

- If  $X$  has density  $f$  and cumulative distribution function  $F$

$$F(x) = \int_{-\infty}^x f(t) dt,$$

then  $F^{-1}(U)$  has the same distribution as  $X$ , where  $U$  is the uniform random variable between 0 and 1 and  $F^{-1}$  is the inverse function of  $F$

$$P(F^{-1}(U) \leq x) = P(U \leq F(x)) = F(x)$$

# Examples

- If  $X$  has exponential distribution with mean  $\frac{1}{3}$ , then

$$F(x) = 1 - e^{-3x}$$

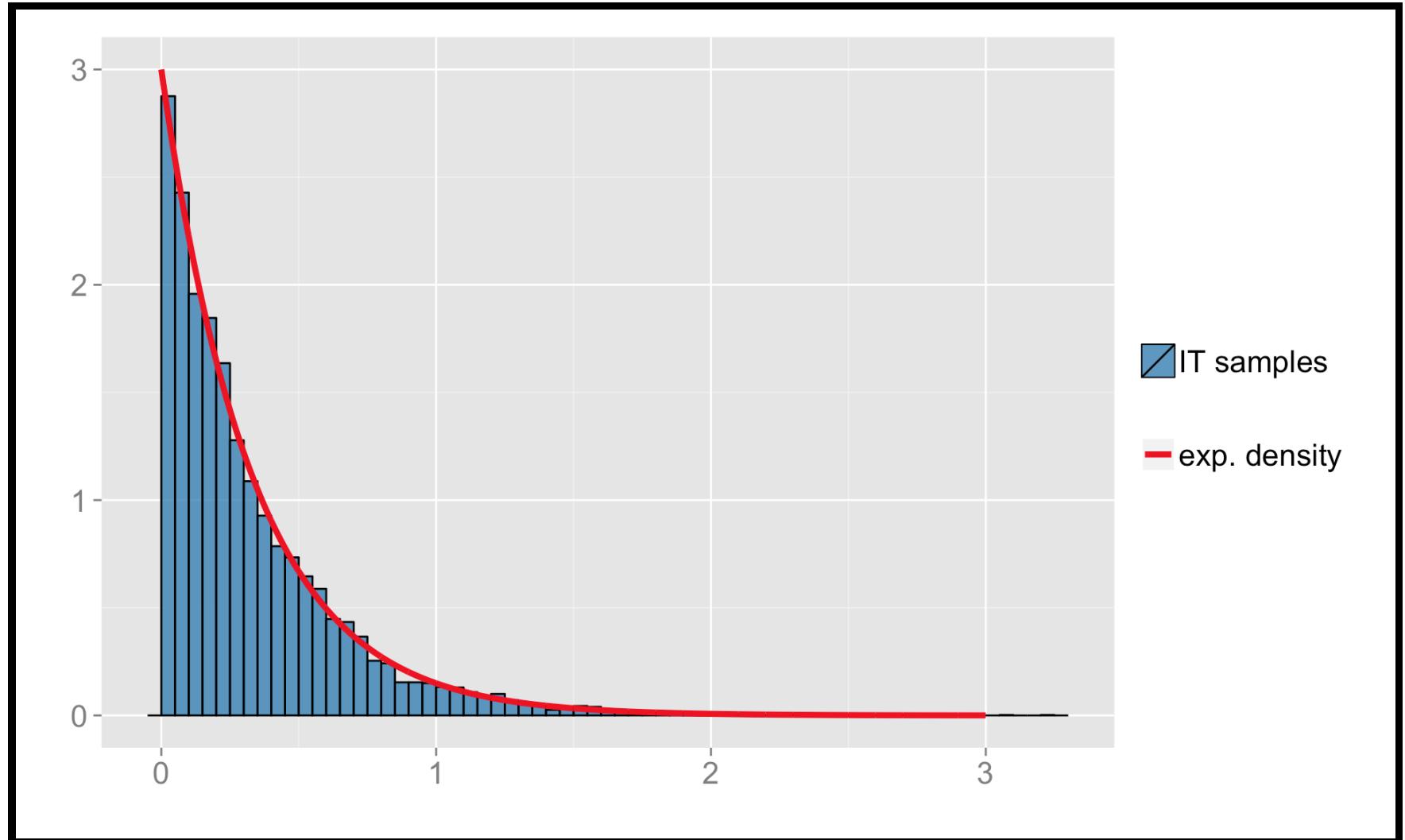
- $F^{-1}(U) = -\frac{1}{3} \log(1 - U)$

```
N <- 10^4; U <- runif(N);  
X <- -log(1 - U) / 3;  
mean(X) ## true mean is 1/3
```

```
## [1] 0.3286
```

```
sd(X) ## true sd is 1/3
```

```
## [1] 0.3286
```



- Cauchy distribution
  - Density:  $f(x) = \frac{1}{\pi(1+x^2)}$
  - CDF:  $F(x) = \frac{1}{2} + \frac{1}{\pi} \arctan(x)$
  - $F^{-1}(u) = \tan\left(\pi\left(u - \frac{1}{2}\right)\right)$
- Pareto distribution
  - Density:  $f(x) = \frac{\alpha}{x^{\alpha+1}}, x \geq 1$
  - CDF:  $F(x) = 1 - \frac{1}{x^\alpha}$
  - $F^{-1}(u) = \frac{1}{(1-u)^{1/\alpha}}$

## Remarks

- Inverse transform method allows us to transform the uniform distribution to *any* other distribution in theory
- However, very often the CDF or its inverse function is difficult or even impossible to compute, in which case we resort other approaches
  - E.g. normal distribution

```
N <- 10^6; U <- runif(N);  
system.time(qnorm(U, mean=0, sd=1))
```

```
##       user   system elapsed  
##  0.041    0.003    0.043
```

```
system.time(rnorm(N, mean=0, sd=1))
```

```
##       user   system elapsed  
##  0.091    0.000    0.092
```

# Acceptance-rejection Method

- **Idea:** if the target distribution is difficult or impossible to directly simulate, then we simulate a simpler distribution and accept only part of the samples based on certain criteria

Given a target density  $f$ , find a density  $g$  and a constant  $M > 0$  such that

$$f(x) \leq Mg(x)$$

for all  $x$  on the support of  $f$

1. Generate  $X$  from  $g$  and  $U$  from Uniform[0,1]
2. If  $U \leq \frac{f(X)}{Mg(X)}$ , accept  $X$
3. Otherwise, reject  $X$  and return to step 1

## Illustration

- Generate a random point  $(X, Mg(X))$  in the region below the function  $Mg(x)$ 
  - $X$  follows density  $g$
- Accept such a point if and only if it is below the function  $f(x)$

# Why?

- The accepted values are *conditioned* values
- Unconditioned  $X$  has density  $g$ , but the accepted  $X$  has density  $f$

$$\begin{aligned} P(X \leq x | \text{accept}) &= \frac{P(X \leq x, U \leq \frac{f(X)}{Mg(X)})}{P(U \leq \frac{f(X)}{Mg(X)})} \\ &= \frac{\int g(t) P(X \leq x, U \leq \frac{f(X)}{Mg(X)} | X = t) dt}{\int g(t) P(U \leq \frac{f(X)}{Mg(X)} | X = t) dt} \\ &= \frac{\int_{-\infty}^x g(t) \frac{f(t)}{Mg(t)} dt}{\int_{-\infty}^{\infty} g(t) \frac{f(t)}{Mg(t)} dt} = \int_{-\infty}^x f(t) dt \end{aligned}$$

## Remarks

- $g$  is often called the *instrumental density*
- An exact upper bound  $M$  is not necessary
- The acceptance rate is  $M^{-1}$ , so the smaller  $M$  the better (more efficient)
  - The efficiency of the method is determined by how closely  $g$  can imitate  $f$ , especially in the tails
- It is necessary for  $g$  to have a “heavier” tail than  $f$ 
  - It is impossible to use the A-R method to simulate a Cauchy distribution using a normal distribution, but the reverse works well

## Example: Normal from Cauchy

- $f$  is a normal density:  $f(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$
- $g$  is a Cauchy density:  $g(x) = \frac{1}{\pi(1+x^2)}$

$$\frac{f(x)}{g(x)} = \sqrt{\frac{\pi}{2}}(1 + x^2)e^{-x^2/2}$$

is maximized at  $x = \pm 1$  and the maximum is  $M = \sqrt{\frac{2\pi}{e}}$

- So the acceptance rate is  $\sqrt{\frac{e}{2\pi}} \approx 0.6577$

```
N <- 10^4  
M <- sqrt(2 * pi/exp(1))  
samples <- rcauchy(N)  
U <- runif(N)  
A_or_R <- U <= dnorm(samples)/(M * dcauchy(samples))  
accepted_samples <- samples[A_or_R]  
mean(accepted_samples)
```

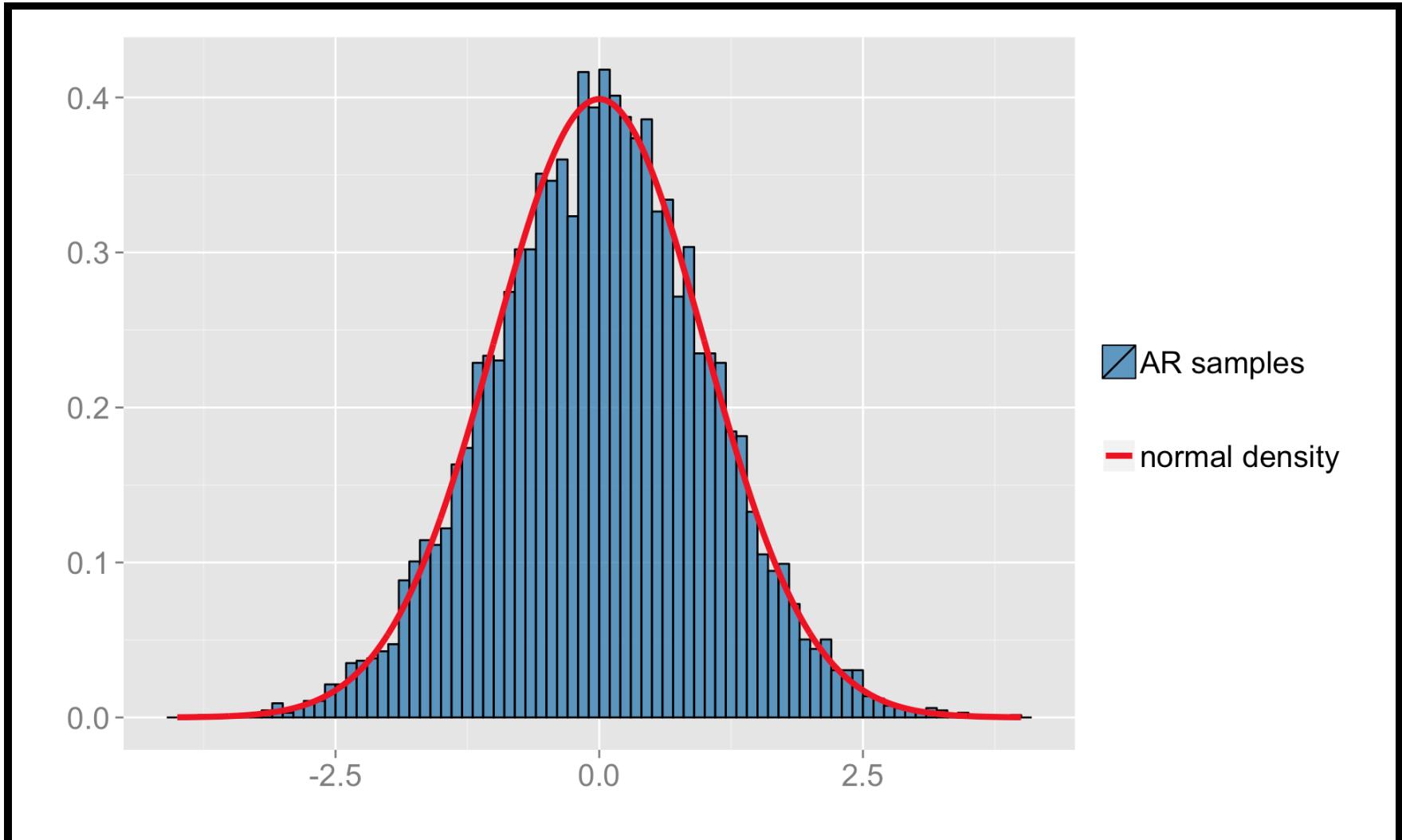
```
## [1] 0.006658
```

```
sd(accepted_samples)
```

```
## [1] 1.014
```

```
length(accepted_samples)/N ## true P(accept) = 0.6577
```

```
## [1] 0.6556
```



## Example: Normal from Doubly Exponential

- Cauchy tail  $x^{-2}$  is much heavier than the normal tail  $e^{-x^2}$
- Try the doubly exponential distribution  $g(x) = \frac{1}{2} e^{-|x|}$ 
  - lighter than Cauchy but is still heavier than normal

$$\frac{f(x)}{g(x)} = \sqrt{\frac{2}{\pi}} e^{|x|-x^2/2}$$

is maximized at  $x = \pm 1$  and the maximum is  $M = \sqrt{\frac{2e}{\pi}}$

- The acceptance rate is  $\sqrt{\frac{\pi}{2e}} \approx 0.7602$ 
  - higher than using Cauchy as the instrumental density

```
N <- 10^4  
M <- sqrt(2 * exp(1)/pi)  
samples <- rexp(N) * sample(c(1, -1), N, replace = TRUE)  
U <- runif(N)  
A_or_R <- U <= dnorm(samples)/(M * 0.5 * dexp(abs(samples)))  
accepted_samples <- samples[A_or_R]  
mean(accepted_samples)
```

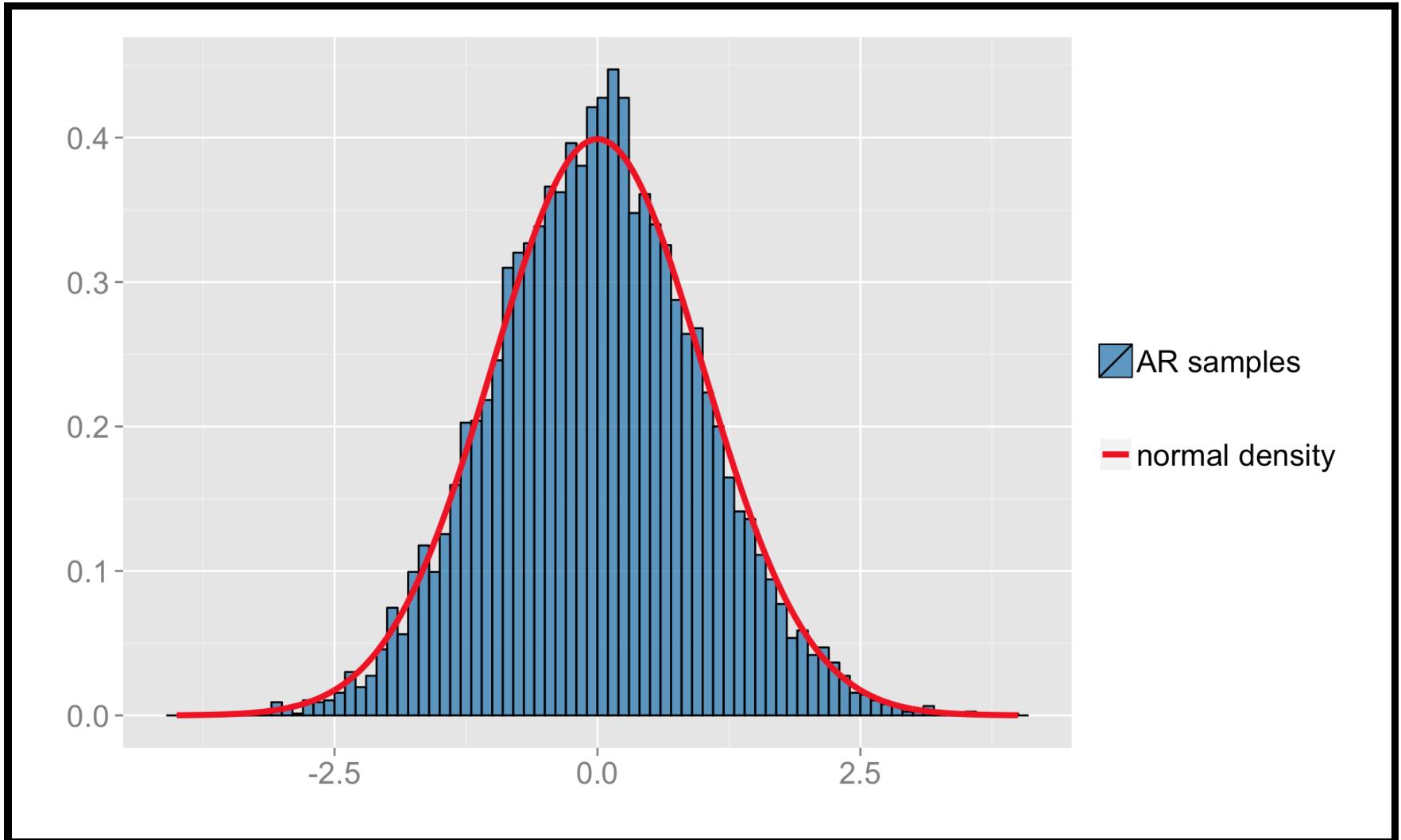
```
## [1] -0.008401
```

```
sd(accepted_samples)
```

```
## [1] 0.9811
```

```
length(accepted_samples)/N ## true P(accept) = 0.7602
```

```
## [1] 0.7648
```



## Example: Beta from Uniform

- $f$  is a beta density:  $f(x) = \frac{x^{a-1}(1-x)^{b-1}}{B(a,b)}$ ,  $0 \leq x \leq 1$ , with  $a, b > 1$
- $g$  is uniform density:  $g(x) = 1$ ,  $0 \leq x \leq 1$

$$\frac{f(x)}{g(x)} = \frac{x^{a-1}(1-x)^{b-1}}{B(a,b)}$$

is maximized at  $x = \frac{a-1}{a+b-2}$  and its maximum is

$$M = \frac{(a-1)^{a-1}(b-1)^{b-1}}{(a+b-2)^{a+b-2}B(a,b)}$$

- Assume  $a = 2.5$  and  $b = 4.2$ . The acceptance rate is 0.4733

```
N <- 10^4
a <- 2.5
b <- 4.2
M <- (a - 1)^(a - 1) * (b - 1)^(b - 1)/(a + b - 2)^(a + b - 2)/beta(a, b)
samples <- runif(N)
U <- runif(N)
A_or_R <- U <= dbeta(samples, a, b)/M
accepted_samples <- samples[A_or_R]
mean(accepted_samples) ## true mean is a/(a+b) = 0.3731
```

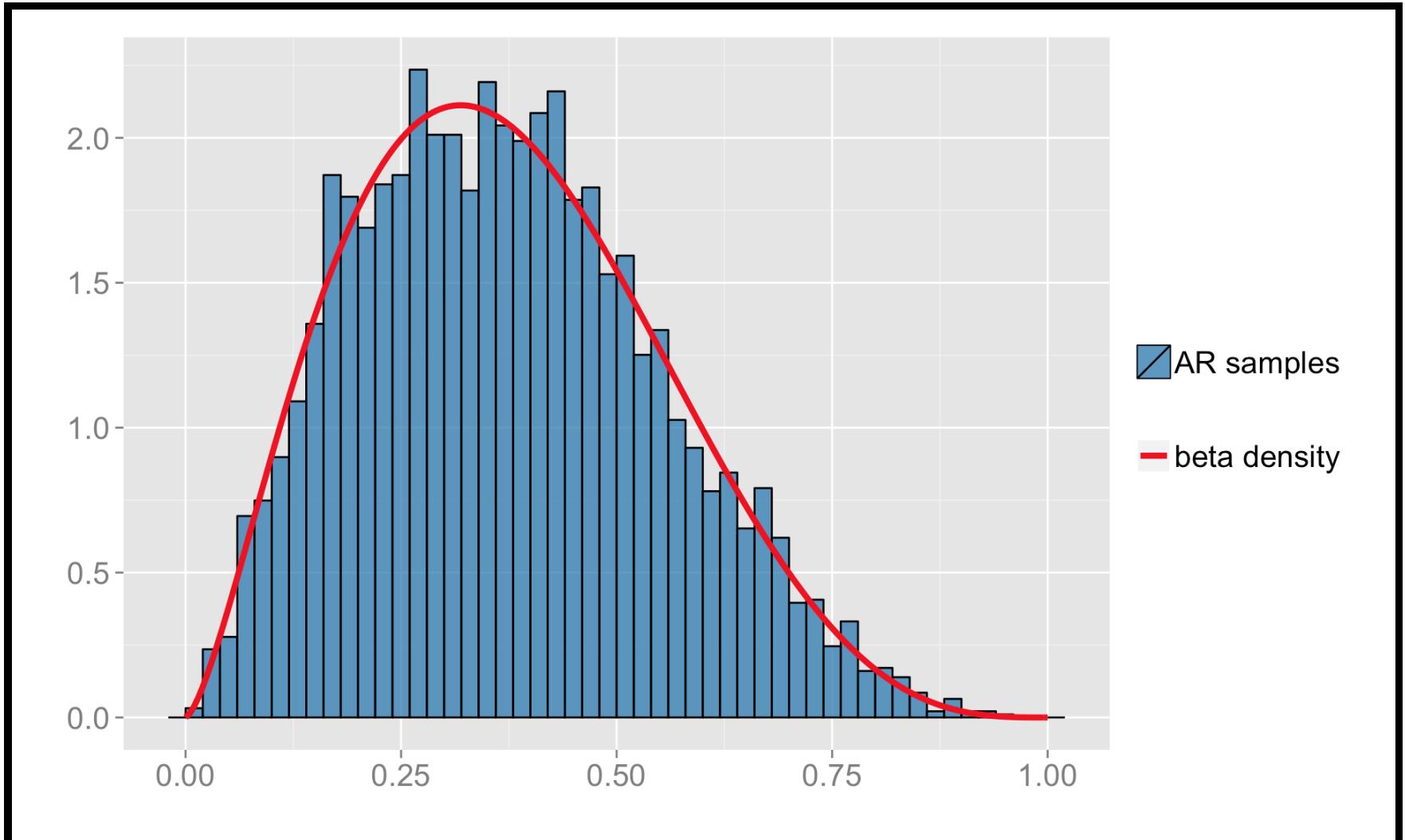
```
## [1] 0.3745
```

```
var(accepted_samples) ## true variance is ab/(a+b)^2/(a+b+1) = 0.0304
```

```
## [1] 0.03065
```

```
length(accepted_samples)/N ## true P(accept) = 0.4733
```

```
## [1] 0.4675
```



## Remarks

- If the target density  $f$  has a *bounded* support, then we can always choose the uniform distribution on the support of  $f$  as the instrumental density
- Then,  $M = \max_x f(x)$

# 5. Markov Chain Monte Carlo

# Introduction

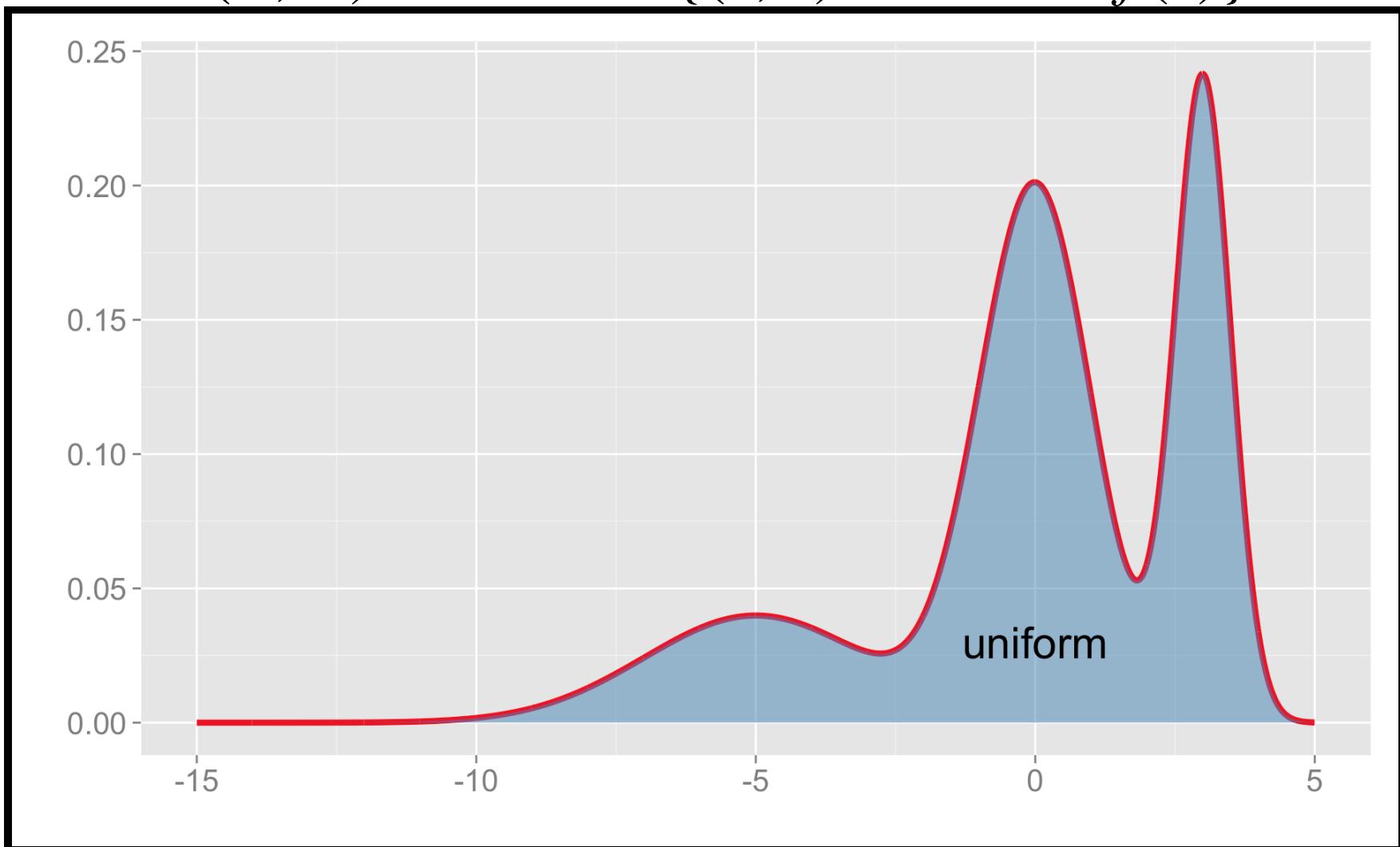
- The posterior distribution in Bayesian statistics is of the form  $p(\theta|y) \propto p(\theta)p(y|\theta)$ 
  - So it is often known up to a normalizing constant, i.e.  
 $p(\theta|y) = Cp(\theta)p(y|\theta)$  for some  $C > 0$  but  $C$  is difficult or impossible to compute
- The basic idea of MCMC is to construct a Markov chain whose *stationary distribution* is the distribution of interest
  - The normalizing constant is not necessary in the process

- The literature on MCMC is enormous
  - *Monte Carlo Statistical Methods*, C. P. Robert and G. Casella, 2nd ed., 2004
- We only introduce three simple MCMC algorithms, but their usage dominates in a great number of applications
  - Slice sampler
  - Metropolis-Hastings algorithm
  - Gibbs sampler

# Slice Sampler

- **Fundamental Theorem of Simulation:** Simulating  $X \sim f(x)$  is equivalent to simulating

$$(X, U) \sim \text{Uniform}\{(x, u) : 0 \leq u \leq f(x)\}$$



## Idea

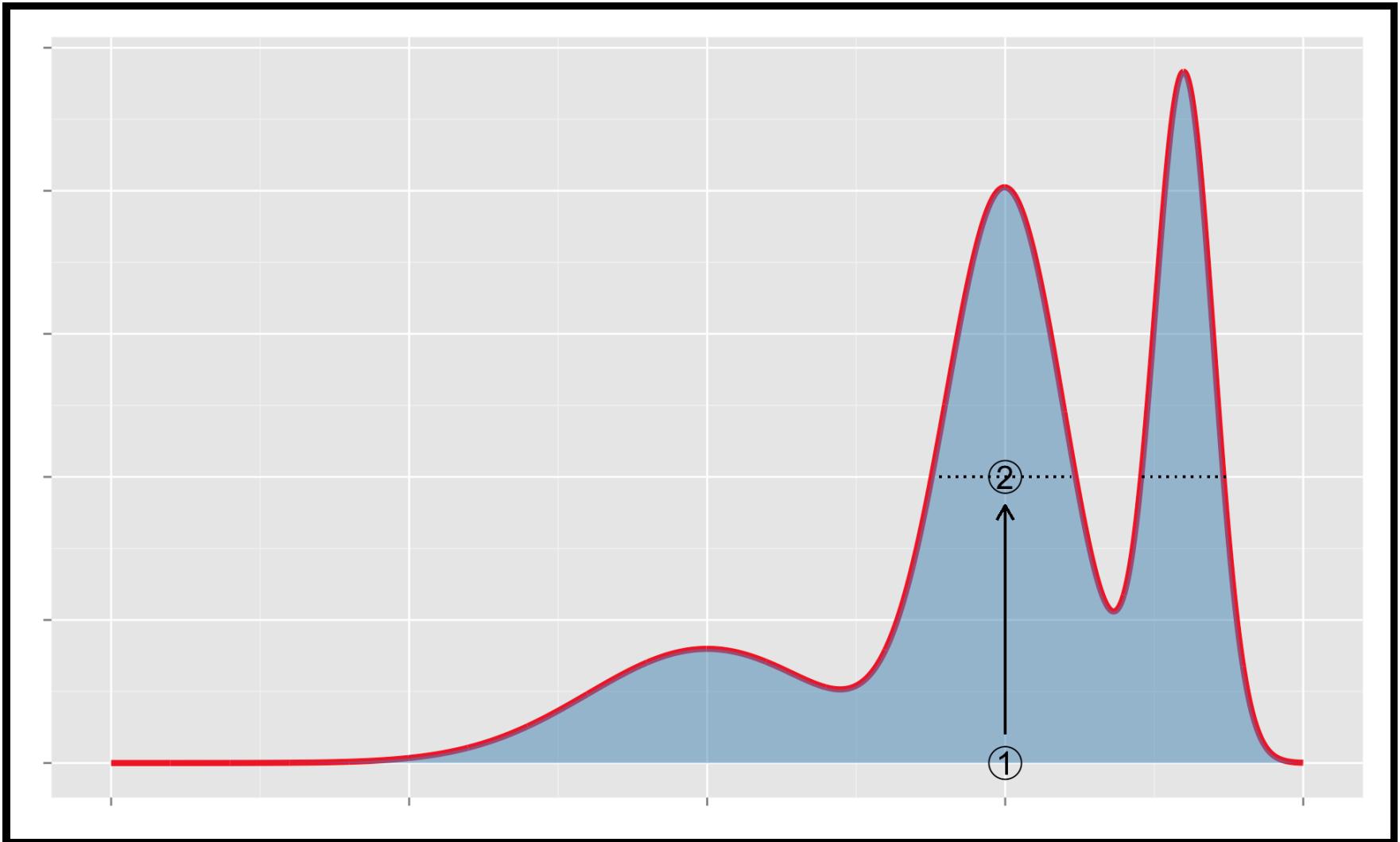
- Construct a *random walk* in the region  $A = \{(x, u) : 0 \leq u \leq f(x)\}$ , whose stationary distribution is the uniform distribution on  $A$ 
  - Do random jumps alternately in vertical and horizontal directions
  - Vertical: uniform on  $\{u : 0 \leq u \leq f(x)\}$
  - Horizontal: uniform on  $\{x : f(x) \geq u\}$ , i.e. “slice”

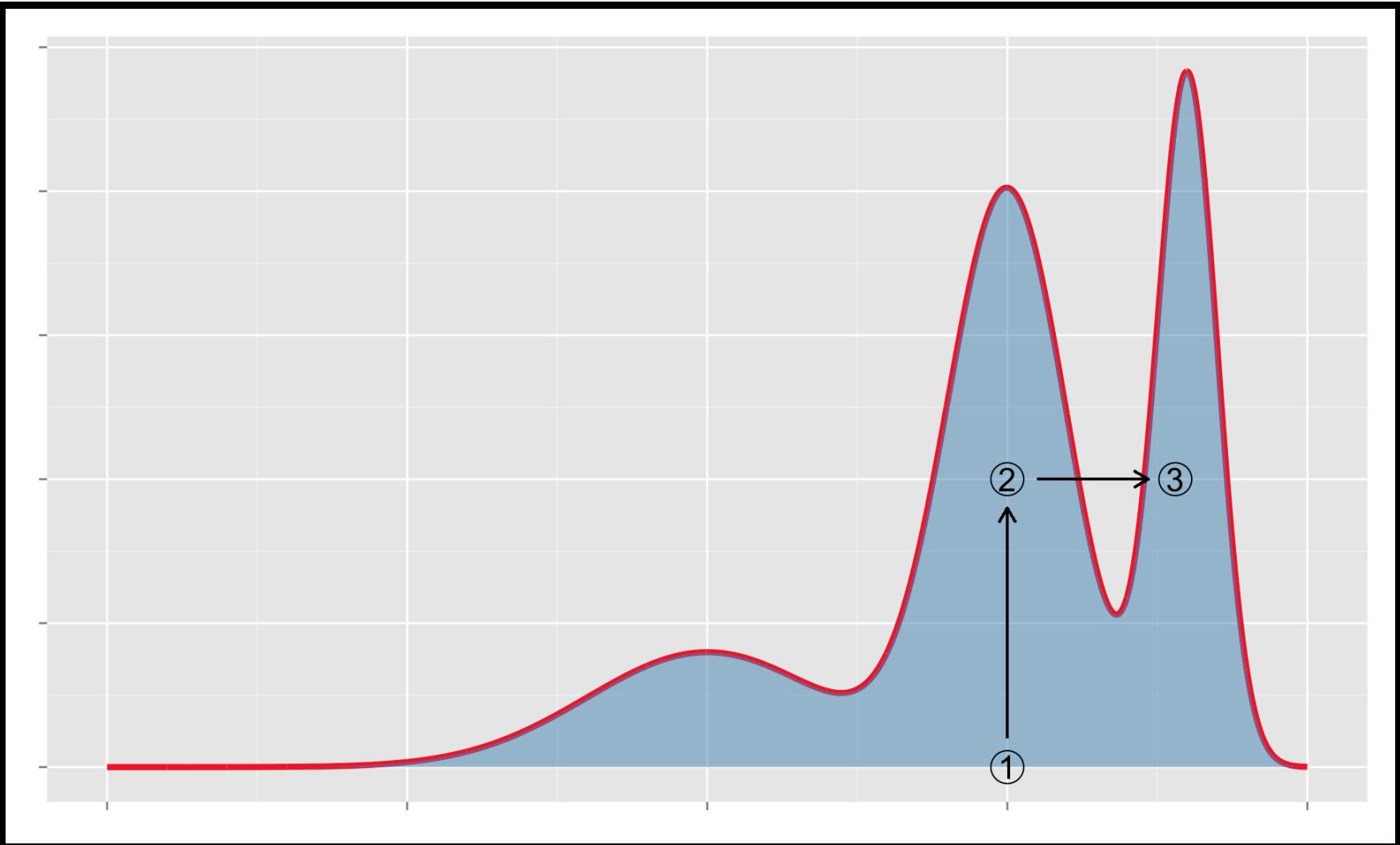
## Slice Sampler Algorithm

For  $t = 1, \dots, T$ , when at  $(x^{(t)}, u^{(t)})$  simulate

1.  $u^{(t+1)} \sim \text{Uniform}(0, f(x^{(t)}))$
2.  $x^{(t+1)} \sim \text{Uniform}(A^{(t+1)})$ , where  
 $A^{(t+1)} = \{x : f(x) \geq u^{(t+1)}\}.$

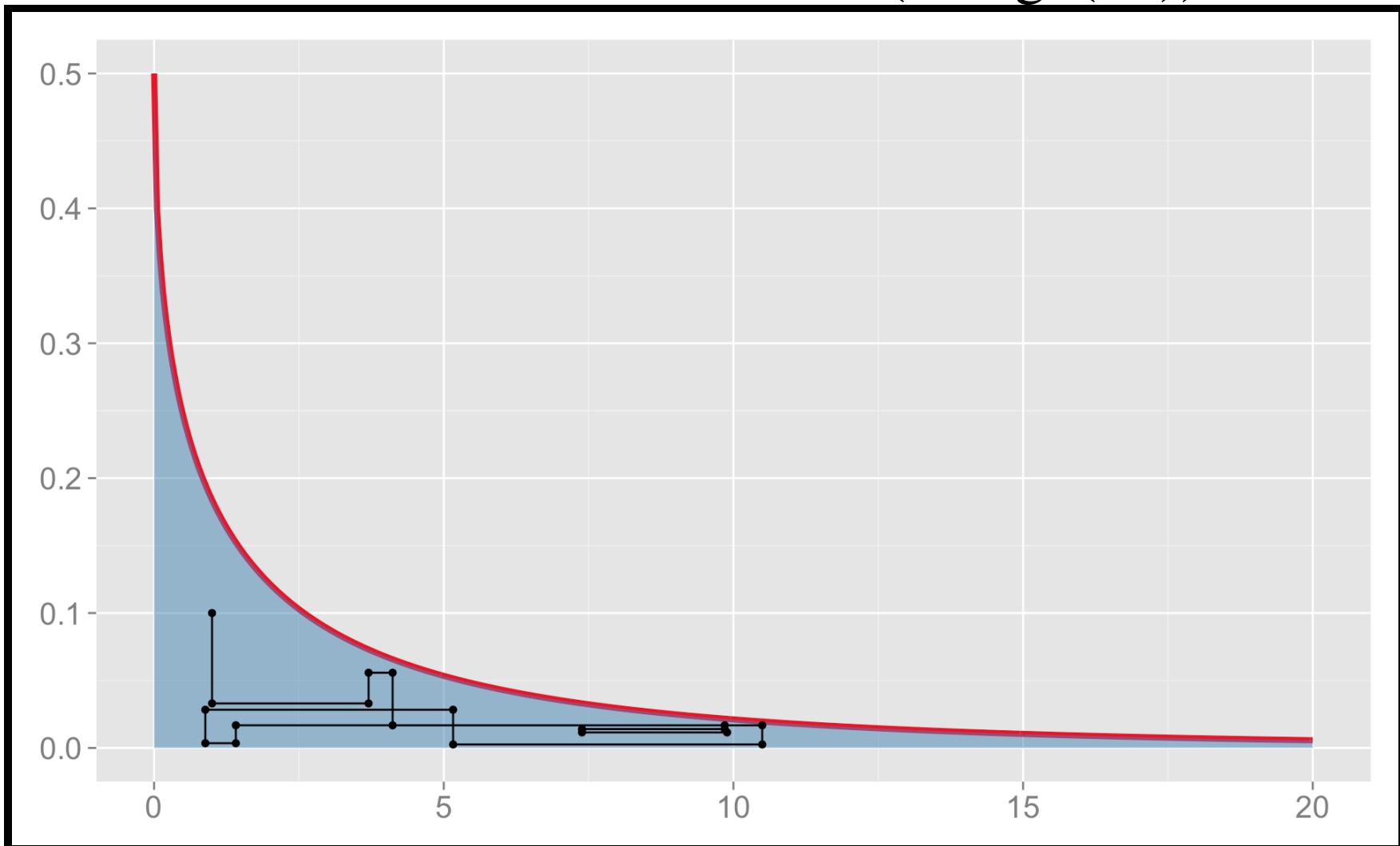
Then,  $\{x^{(t)} : t = 1, \dots, T\}$  are samples generated from  $f(x)$





## Example 1

- Target density  $f(x) = \frac{1}{2} e^{-\sqrt{x}}, x \geq 0$
- Vertical:  $U|x \sim \text{Uniform}(0, \frac{1}{2} e^{-\sqrt{x}})$
- Horizontal:  $X|u \sim \text{Uniform}(0, \log^2(2u))$



```
T <- 10^4
x <- rep(1, T)
y <- rep(0.1, T)
for (t in 1:(T - 1)) {
  y[t + 1] <- runif(1, 0, exp(-sqrt(x[t]))/2)
  x[t + 1] <- runif(1, 0, (log(2 * y[t + 1])))^2)
}
```

## Example 2 (Truncated Normal)

- Target density:  $f(x) \propto f_1(x) = e^{-(x+3)^2/2} \mathbb{I}_{[0,1]}(x)$
- Vertical:  $U|x \sim \text{Uniform}(0, e^{-(x+3)^2/2})$
- Horizontal:  $X|u \sim \text{Uniform}(0, \min(1, \sqrt{-2 \log(u)} - 3))$

```
T <- 10^4
x <- rep(0.25, T)
y <- rep(0.0025, T)
for (t in 1:(T - 1)) {
  y[t + 1] <- runif(1, 0, exp(-(x[t] + 3)^2/2))
  x[t + 1] <- runif(1, 0, min(1, sqrt(-2 * log(y[t + 1]))) - 3))
}
```

## Remarks

- $\{x^{(t)} : t = 1, \dots, T\}$  form a Markov chain and its stationary distribution has the target density  $f(x)$
- Advantage: it does not need an instrumental distribution or the normalizing constant of the target distribution
- Disadvantage: it may be difficult to compute the region  $\{x : f(x) \geq u\}$ , especially for multi-dimensional cases

# Metropolis-Hastings Algorithm

- Metropolis algorithm was proposed in 1953
- Hastings generalized the algorithm in 1970 and introduced it to the statistics community
- Generate a sequence of samples that form a Markov chain whose stationary distribution is the target distribution
  - The next sample value is dependent only on the current sample value
  - At each iteration, a candidate is proposed from a simple distribution and then an acceptance-rejection step is done

- Similar as the acceptance-rejection method, the MH algorithm requires an *instrumental* distribution  $q(y|x)$  that is easy to simulate from

For  $t = 1, \dots, T$ , when at  $x^{(t)}$

1. Simulate  $y_t \sim q(y|x^{(t)})$
2. Simulate  $U \sim \text{Uniform}(0, 1)$  and take

$$x^{(t+1)} = \begin{cases} y_t, & \text{if } U \leq \frac{f(y_t)}{f(x^{(t)})} \frac{q(x^{(t)}|y_t)}{q(y_t|x^{(t)})} \\ x^{(t)}, & \text{otherwise.} \end{cases}$$

## Remarks

- $x^{(1)}, x^{(2)}, \dots$  are correlated
- The chain may take the same value several times in a row
  - Possibly gets stuck if the acceptance rate is too low
- The warm-up period must be discarded to alleviate the initialization bias
  - E.g., discard  $\{x^{(t)} : t = 1, \dots, \tau\}$  and only use  $\{x^{(t)} : t = \tau + 1, \dots, T\}$  to approximate the target distribution

- Never move to values with  $f(y) = 0$
- Only depends on ratios  $f(y)/f(x)$  and  $q(x|y)/q(y|x)$ 
  - Independent of normalizing constants
- Always accepts  $y_t$  such that

$$\frac{f(y_t)}{q(y_t|x^{(t)})} > \frac{f(x^{(t)})}{q(x^{(t)}|y_t)}$$

- If  $y_t$  decreases the ratio, it is sometimes rejected but may still be accepted
- There are two typical variants
  - Independent MH
  - Random walk MH

## Independent Metropolis-Hastings

- Instrumental distribution  $q$  is independent of the current position  $x^{(t)}$ , i.e.  $q(y|x) = g(y)$

For  $t = 1, \dots, T$ , when at  $x^{(t)}$

1. Simulate  $y_t \sim g(y)$
  2. Simulate  $U \sim \text{Uniform}(0, 1)$  and take
- $$x^{(t+1)} = \begin{cases} y_t, & \text{if } U \leq \frac{f(y_t)}{f(x^{(t)})} \frac{g(x^{(t)})}{g(y_t)} \\ x^{(t)}, & \text{otherwise.} \end{cases}$$

## Remarks

- Can be viewed as a generalization of the Acceptance-Rejection method
- The A-R sample is i.i.d., whereas the MH sample is correlated
- The A-R acceptance step requires the calculation of  $M$  (i.e.  $f(x) \leq Mg(x)$ ), where MH does not
  - Independent MH is A-R “for lazy people”
- It can be shown that if  $f(x) \leq Mg(x)$ , then the acceptance rate of independent MH is at least  $1/M$ 
  - So independent MH accepts more proposed samples than A-R at the cost of losing independence among samples

# Example

- Target:  $f(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$
- Instrumental:  $g(x) = \frac{1}{2} e^{-|x|}$
- The acceptance probability in independent MH is  $\min\{1, \exp[(|x^{(t)}| - |y_t|)((|x^{(t)}| + |y_t|)/2 - 1)]\}$

```
N <- 10^4; x <- rep(0, N); accept_count <- 0;
y <- rexp(N) * sample(c(1, -1), size=N, replace=TRUE) ## simulate double exp.
U <- runif(N)
for (t in 1:(N-1)){
  if (U[t] <= exp((abs(x[t])-abs(y[t])) * ((abs(x[t]+abs(y[t])))/2-1))){
    accept_count <- accept_count + 1
    x[t+1] <- y[t]
  }
  else
    x[t+1] <- x[t]
}
accept_count / N ## acceptance rate for A-R is 0.7602
## [1] 0.8402
```

- Despite of more efficient use of proposed samples (higher acceptance rate), the MH sample approximates the target distribution worse than the A-R samples
  - A-R is exact, while MH needs the Markov chain to converge to the target distribution and any finite sample is merely an approximation
  - “Penalty for being lazy!”

## Random Walk Metropolis-Hastings

- This is the original algorithm in Metropolis et al. (1953), thus called the Metropolis algorithm
- Independent MH is sometimes difficult to implement
  - Construction of instrumental distribution may be difficult
  - Instrumental distribution is a *global* proposal and ignores *local* information:  $q(y|x)$  is independent of  $x$

- Simulate  $y_t = x^{(t)} + \epsilon_t$ , where  $\epsilon_t$  is random perturbation
    - $\epsilon_t$  independent of  $x^{(t)}$ , having a symmetric distribution  $g$  with mean 0
  - Instrumental distribution  $q(y|x) = g(y - x)$
- For  $t = 1, \dots, T$ , when at  $x^{(t)}$

1. Simulate  $y_t \sim g(y - x^{(t)})$
2. Simulate  $U \sim \text{Uniform}(0, 1)$  and take

$$x^{(t+1)} = \begin{cases} y_t, & \text{if } U \leq \frac{f(y_t)}{f(x^{(t)})} \\ x^{(t)}, & \text{otherwise.} \end{cases}$$

## Remarks

- Given a proposed candidate  $y_t$ , its acceptance probability is independent of  $g$
- However, the overall acceptance rate of the algorithm does depend on  $g$ 
  - It determines how the algorithm explores the state space to propose candidates

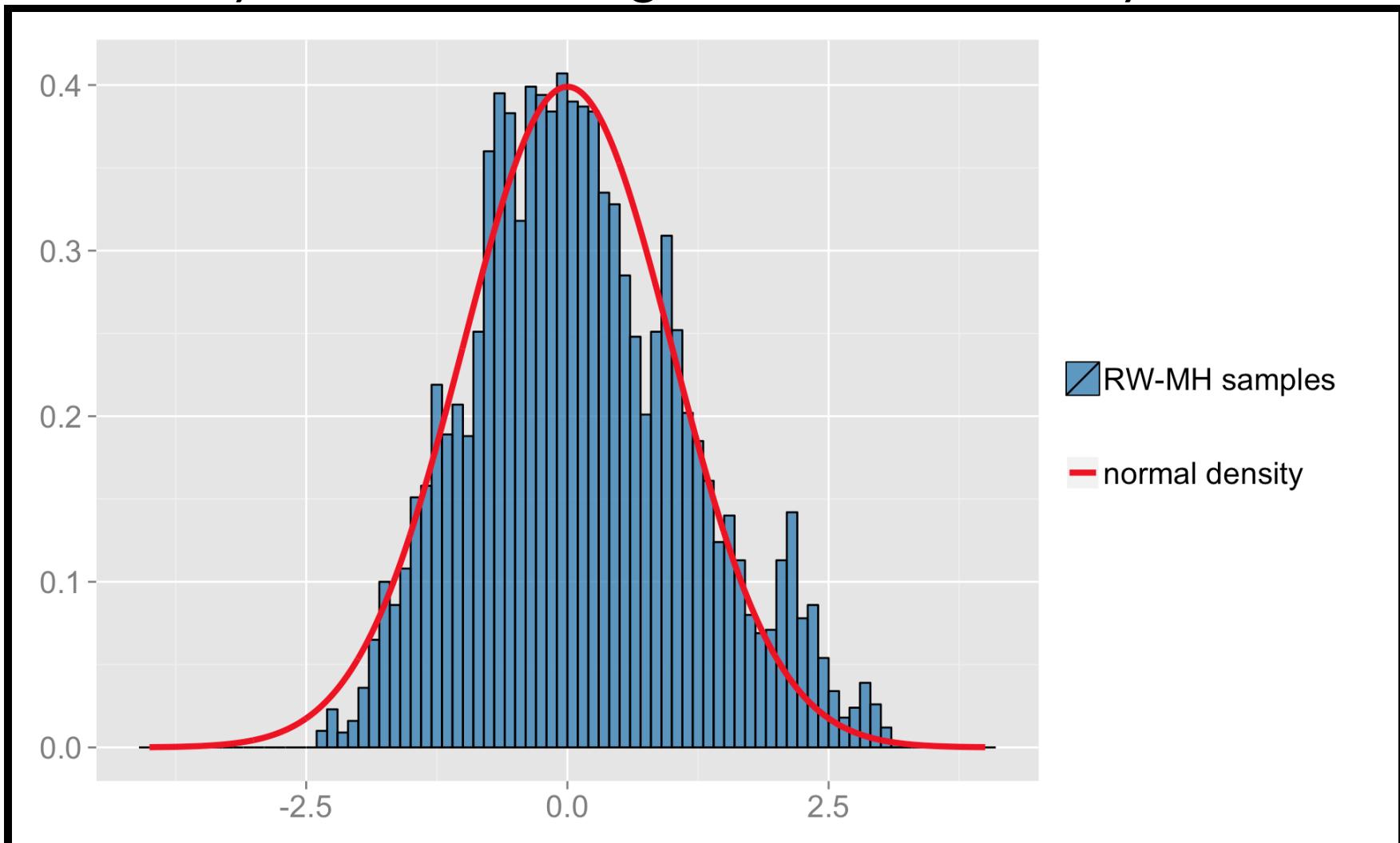
- If a candidate is a more probable than the current point (i.e.  $f(y_t) \geq f(x^{(t)})$ ), then we *always* accept the move
- Otherwise, we *sometimes* reject the move; the more relative drop in likelihood, the more likely we are to reject the move
- So in the long run, the chain tends to stay in high-density regions of  $f(x)$ , while occasionally visiting low-density regions

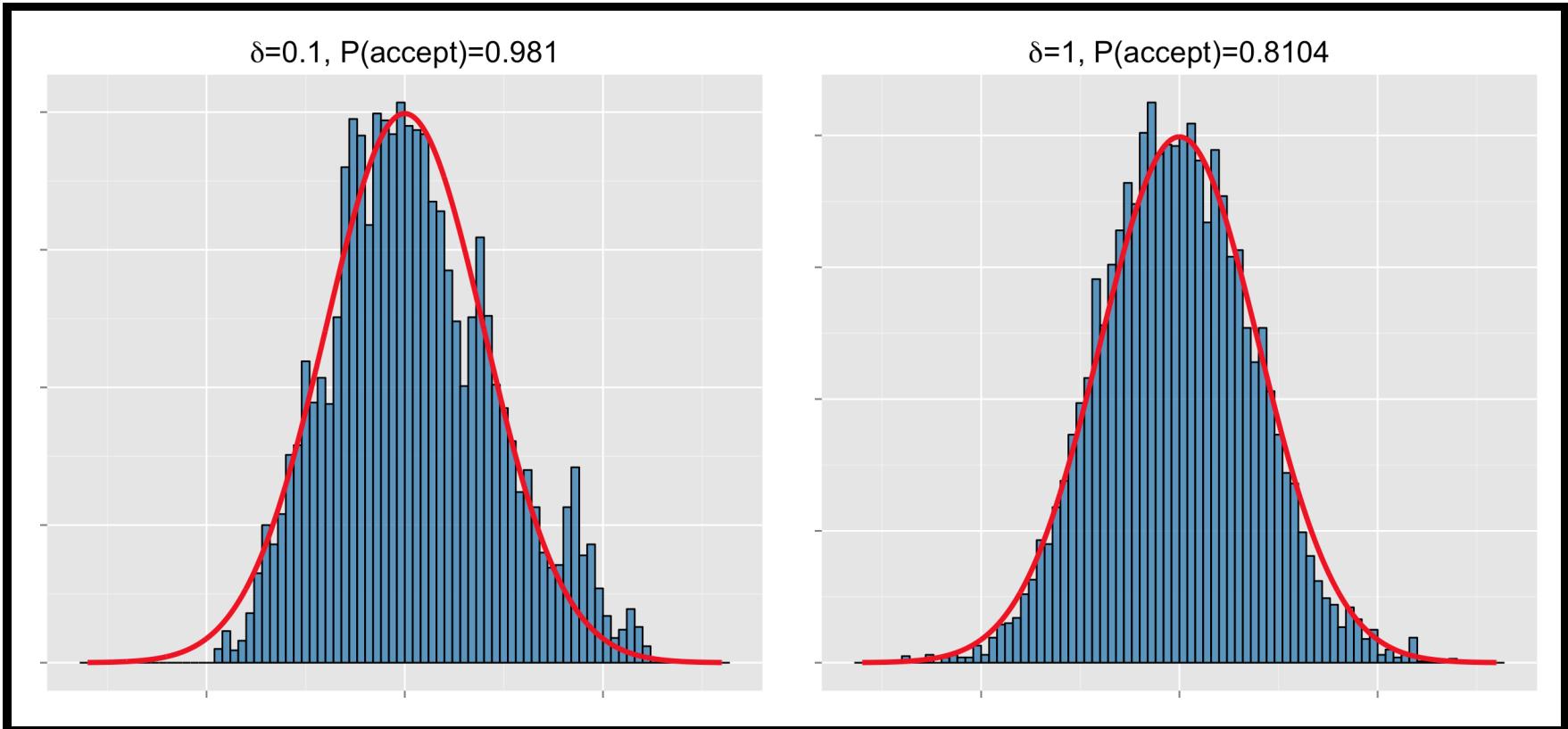
## Example

- Target:  $f(x) = \frac{1}{2} e^{-x^2/2}$
- Instrumental:  $g(x) = \frac{1}{2\delta}$  for  $x \in [-\delta, \delta]$
- $\delta$  controls the “scale” of the random walk
  - small  $\delta$  means high acceptance rate
- The acceptance probability in random walk MH is
$$\min\{1, \exp[(x^{(t)})^2 - y_t^2]/2\}$$

```
N <- 10^4; x <- rep(0, N); delta <- 0.1; accept_count <- 0;
epsilon <- runif(N, -delta, delta) ## simulate uniform on [-delta, delta]
U <- runif(N)
for (t in 1:(N-1)){
  y_t <- x[t] + epsilon[t]
  if (U[t] <= exp((x[t]^2 - y_t^2)/2)){
    accept_count <- accept_count + 1
    x[t+1] <- y_t
  }
  else
    x[t+1] <- x[t]
}
accept_count / N; ## maybe too high...
## [1] 0.981
```

- Unlike the acceptance-rejection method, having a high acceptance rate is not necessarily desirable for random walk MH.
  - It may lead to poor exploration of the tails of the target density and slow convergence to the stationary distribution





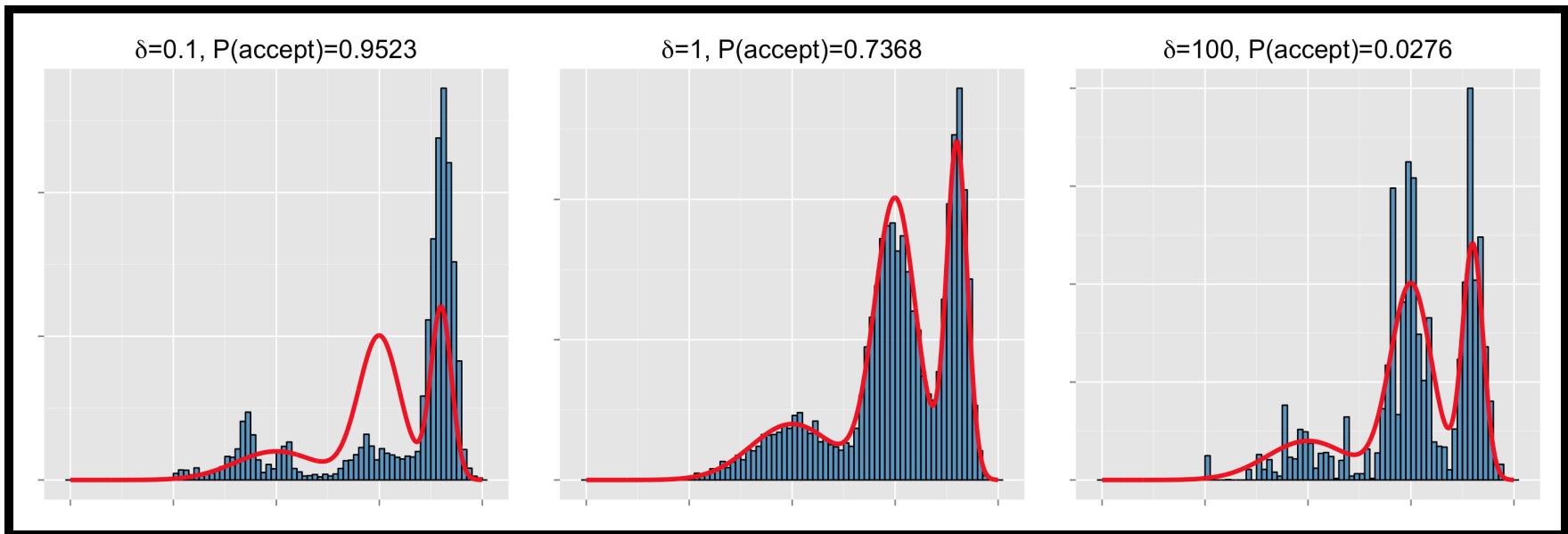
Though the acceptance rate is lower, we get a better histogram  
for a larger value of  $\delta$

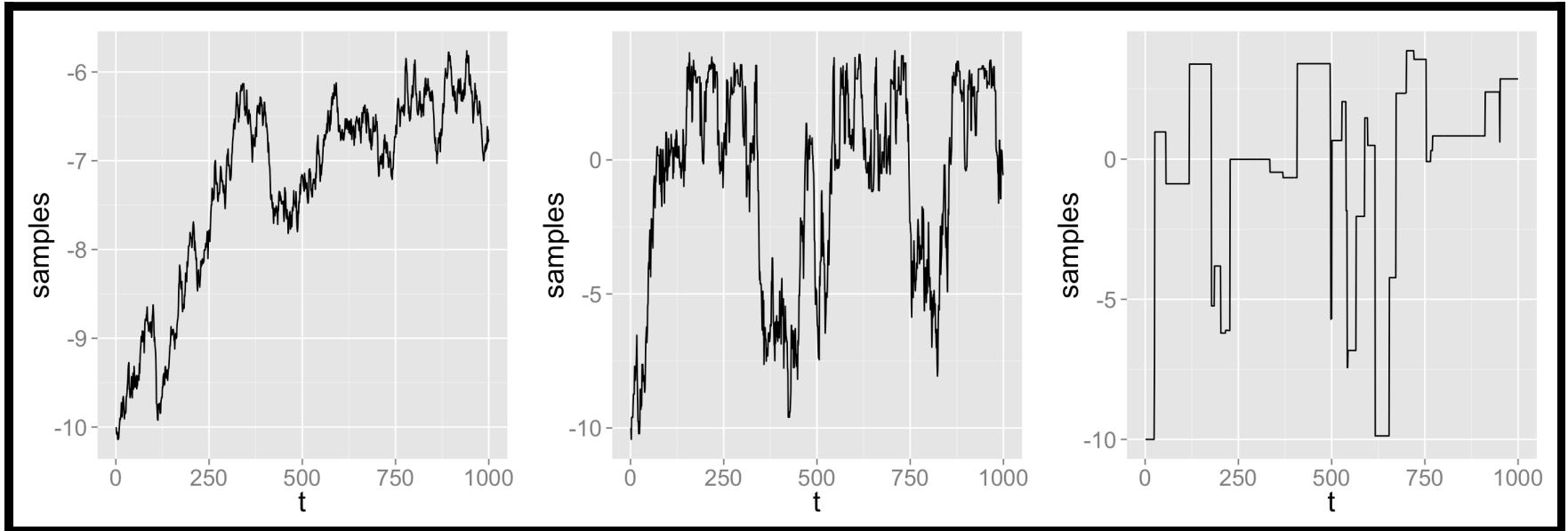
# Optimizing Acceptance Rate

- How do we choose the instrumental distribution  $q$  when developing a MH algorithm?
- A criterion is the acceptance rate
  - It can be easily estimated by the empirical frequency of acceptance
- In contrast to the A-R method, maximizing the acceptance rate is not necessarily the best, especially for random walk MH

- For independent MH, we can optimize the algorithm by maximizing acceptance rate
- For random walk MH, it gets more complicated...
  - If the acceptance rate is high, the random walk is moving too slowly on the surface of  $f$ , and it may get stuck in a high-density region
  - If the acceptance rate is low, the random walk is moving too quickly on the surface of  $f$ , and it may miss an important but isolated mode of  $f$
  - Nevertheless, a low acceptance rate is less of an issue

- Target is a normal mixture  
 $0.2\mathcal{N}(-5, 4) + 0.5\mathcal{N}(0, 1) + 0.3\mathcal{N}(3, 0.25)$
- Instrumental is normal with mean 0 and sd  $\delta$  for RW-MH





- Gelman, Gilks and Roberts (1995) suggested:

*In small dimensions, aim at an average acceptance rate of 50%. In large dimensions, at an average acceptance rate of 25%.*

# Gibbs Sampler

- Proposed by S. Geman and D. Geman in 1984
- Named after the physicist J. Gibbs in reference to an analogy between the algorithm and statistical physics
- Used to simulate a *multivariate* distribution
  - Decompose joint distribution into a sequence of one-dimensional conditional distributions

- Target  $f$  is the joint distribution of  $\mathbf{X} = (X_1, \dots, X_n)$

- Suppose we can simulate from the *full conditionals*

$$X_i | \mathbf{x}_{-i} \sim f_i(x_i | \mathbf{x}_{-i})$$

for  $i = 1, \dots, n$ , where  $\mathbf{x}_{-i} = (x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)$

- Then we can construct a Markov chain  $\{\mathbf{X}^{(t)}\}$  whose stationary distribution is  $f$

For  $t = 1, \dots, T$ , given  $\mathbf{x}^{(t)} = (x_1^{(t)}, \dots, x_n^{(t)})$ , simulate

- $X_1^{(t+1)} \sim f_1(x_1 | \mathbf{x}_2^{(t)}, \mathbf{x}_3^{(t)}, \dots, \mathbf{x}_n^{(t)})$
- $X_2^{(t+1)} \sim f_2(x_2 | \mathbf{x}_1^{(t+1)}, \mathbf{x}_3^{(t)}, \dots, \mathbf{x}_n^{(t)})$
- ⋮
- $X_n^{(t+1)} \sim f_n(x_n | \mathbf{x}_1^{(t+1)}, \mathbf{x}_2^{(t+1)}, \dots, \mathbf{x}_{n-1}^{(t+1)})$

## Example

- Target is  $f(x, y) \propto e^{-(x^2y^2+x^2+y^2-8x-8y)/2}$
- The full conditionals are

$$f(x|y) \propto e^{-[(y^2+1)x^2-8x]/2}$$

and

$$f(y|x) \propto e^{-[(x^2+1)y^2-8y]/2}$$

- Noting the quadratic form in the exponent, the full conditionals are simply normal distributions

$$x|y \sim \mathcal{N}\left(4/(1 + y^2), 1/(1 + y^2)\right)$$

and

$$y|x \sim \mathcal{N}\left(4/(1 + x^2), 1/(1 + x^2)\right)$$

```
N <- 10^4; x <- rep(0, N); y <- rep(0, N);
for (t in 1:(N-1)){
  x[t+1] <- rnorm(1, mean=4/(1+y[t]^2), sd=1/sqrt(1+y[t]^2))
  y[t+1] <- rnorm(1, mean=4/(1+x[t+1]^2), sd=1/sqrt(1+x[t+1]^2))
}
```

# Summary

- Slice sampler does not need an instrumental distribution but requires one to compute the “inverse” of the density function
- Metropolis-Hastings requires carefully choosing an instrumental distribution
  - Independent MH: instrumental density should have “heavier” tails (similar as A-R method) than the target density to guarantee convergence; it can be optimized by maximizing acceptance rate
  - Random walk MH: more complicated... high acceptance rate is not necessarily desirable and low acceptance rate is less of an issue
- Gibbs sampler converts a multi-dimensional distribution to a sequence of one-dimensional conditional distributions (i.e. full conditionals)

# 6. An Application in Finance

# Background

- Companies may default especially in a bad economy
- $N(t)$  is the accumulated number of defaults since time 0
- $x(t)$  is the “state” of the economy, which can not be observed directly

- $N(t)$  can be modeled as doubly stochastic Poisson process with arrival rate  $\lambda(t)$ 
  - Conditional on  $\{\lambda(t) : 0 \leq t \leq T\}, \{N(t) : 0 \leq t \leq T\}$  is an inhomogeneous Poisson process, i.e.  $N(t)$  has a Poisson distribution with mean  $\int_0^t \lambda(s) ds$
- Assume  $\lambda(t) = \mu e^{x(t)}$  and  

$$dx(t) = -x(t)dt + \sigma dW(t),$$
where  $W(t)$  is a standard Brownian motion
- We are concerned with the estimation of the parameters  
 $\Theta = (\mu, \kappa, \sigma)$

- This model can be discretized into a *state space* model

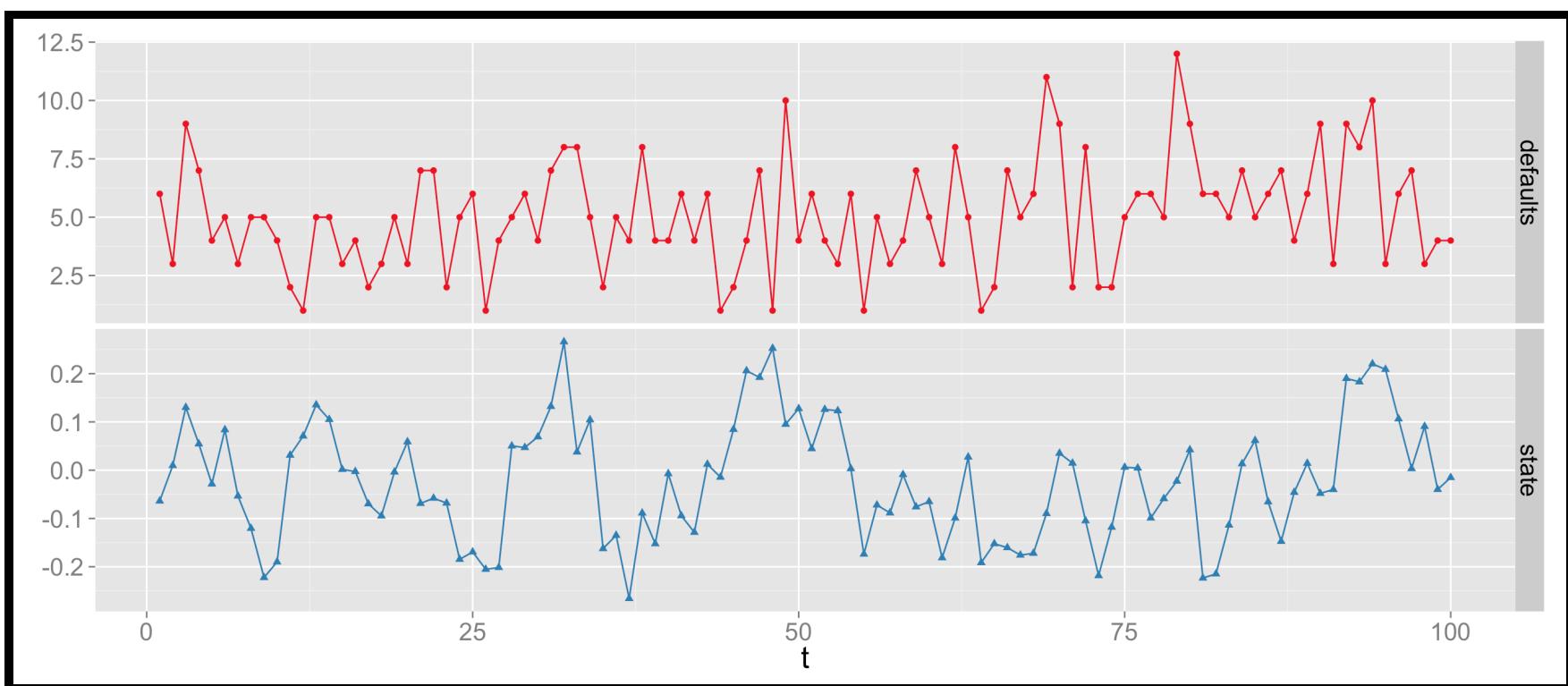
$$\begin{cases} Y_t | x_t, \Theta \sim \text{Poisson}(\mu e^{x_t}) \\ x_t | x_{t-1}, \Theta \sim \text{Normal}((1 - \kappa)x_{t-1}, \sigma^2) \end{cases}$$

where  $Y_t = N(t) - N(t - 1)$  is the number of defaults during  $[t - 1, t]$

```

T <- 100;
kappa <- 0.3; sigma <- 0.1; mu <- 5;
x_0 <- 0;
x <- rep(x_0, T+1);
for (t in 1:T)
  x[t+1] <- rnorm(1, mean=(1-kappa)*x[t], sd=sigma)
y <- rpois(T, mu*exp(x[2:(T+1)]))

```



- A challenge here, and also for other state space models, is that the “states” are unobservable (i.e. latent variables)
- Maximum likelihood estimation typically fails for state space models because all the latent variables must be “integrated out” in order to compute the likelihood function
  - Exceptions include linear Gaussian models and hidden Markov chains with finite state space
- Given the data  $\mathbf{Y} = \{Y_1, \dots, Y_T\}$ , Bayesian inference is interested in the joint posterior distribution of the parameters  $\Theta$  and the state variables  $\mathbf{x} = (x_1, \dots, x_T)$   

$$p(\Theta, \mathbf{x}|\mathbf{Y})$$

# Bayesian Analysis

- Gibbs sampler indicates we can simulate full conditionals
  - $p(\mu|\kappa, \sigma^2, \mathbf{x}, \mathbf{Y})$
  - $p(\kappa|\mu, \sigma^2, \mathbf{x}, \mathbf{Y})$
  - $p(\sigma^2|\mu, \kappa, \mathbf{x}, \mathbf{Y})$
  - $p(x_t|\mu, \kappa, \sigma^2, \mathbf{x}_{-t}, \mathbf{Y}), t = 1, \dots, T$
- Conjugate priors can be found for the first three but the last one needs Metropolis-Hastings

- We first write down the *complete likelihood*  $p(\mathbf{Y}, \mathbf{x}|\Theta)$

$$p(\mathbf{Y}, \mathbf{x}|\Theta) = \prod_{t=1}^T p(Y_t|x_t, \mu)p(x_t|x_{t-1}, \kappa, \sigma^2)$$

$$\propto \prod_{t=1}^T (\mu e^{x_t})^{Y_t} e^{-\mu e^{x_t}} \cdot e^{-[x_t - (1-\kappa)x_{t-1}]^2/(2\sigma^2)}$$

where

$$p(Y_t|x_t, \mu) = \frac{(\mu e^{x_t})^{Y_t}}{Y_t!} e^{-\mu e^{x_t}}$$

and

$$p(x_t|x_{t-1}, \kappa, \sigma^2) = \frac{1}{2\sigma^2} e^{-[x_t - (1-\kappa)x_{t-1}]^2/(2\sigma^2)}$$

- Assume the priors of the parameters are independent
  - Assume  $p(\mu)$  is Gamma with shape  $a_1$  and rate  $b_1$ ,
- $$p(\mu|\kappa, \sigma^2, \mathbf{x}, \mathbf{Y}) \propto p(\mu|\kappa, \sigma^2)p(\mathbf{Y}, \mathbf{x}|\mu, \kappa, \sigma^2)$$

$$\begin{aligned} & \propto p(\mu) \prod_{t=1}^T p(Y_t|x_t, \mu) \\ & \propto \mu^{a_1-1} e^{-b_1\mu} \prod_{t=1}^T (\mu e^{x_t})^{Y_t} e^{-\mu e^{x_t}} \\ & \propto \mu^{a_1-1 + \sum_t Y_t} \cdot e^{-\mu(b_1 + \sum_t e^{x_t})} \end{aligned}$$

so  $p(\mu|\kappa, \sigma^2, \mathbf{x}, \mathbf{Y})$  is Gamma with shape  $a_1 + \sum_t Y_t$  and rate  $b_1 + \sum_t e^{x_t}$

## Exercise 1

Assume  $p(\kappa)$  is normal with mean  $a_2$  and variance  $b_2^2$ . Then  $p(\kappa|\mu, \sigma^2, \mathbf{x}, \mathbf{Y})$  is normal with mean  $B/A$  and variance  $1/A$ , where

$$A = 1/b_2^2 + \sum_t x_t^2/\sigma^2$$

and

$$B = a_2/b_2^2 - \sum_t x_{t-1}(x_t - x_{t-1})/\sigma^2$$

## Exercise 2

Assume  $p(\sigma^2)$  is inverse Gamma (i.e.  $p(1/\sigma^2)$  is Gamma) with shape  $a_3$  and rate  $b_3$ . Then  $p(\sigma^2|\mu, \kappa, \mathbf{x}, \mathbf{Y})$  is inverse Gamma with shape  $a_3 + T/2$  and scale

$$b_3 + \sum_t [x_t - (1 - \kappa)x_{t-1}]^2/2$$

## Exercise 3

$p(x_t | \mathbf{x}_{-t}, \mathbf{Y}, \Theta) \propto p(x_{t+1} | x_t, \Theta)p(x_t | x_{t-1}, \Theta)p(Y_t | x_t, \Theta),$   
where

$$p(x_{t+1} | x_t, \Theta) \propto \exp\left(-\frac{[x_{t+1} - (1-\kappa)x_t]^2}{2\sigma^2}\right)$$

$$p(x_t | x_{t-1}, \Theta) \propto \exp\left(-\frac{[x_t - (1-\kappa)x_{t-1}]^2}{2\sigma^2}\right)$$

$$p(Y_t | x_t, \Theta) \propto \exp(-\mu e^{x_t} + x_t Y_t)$$

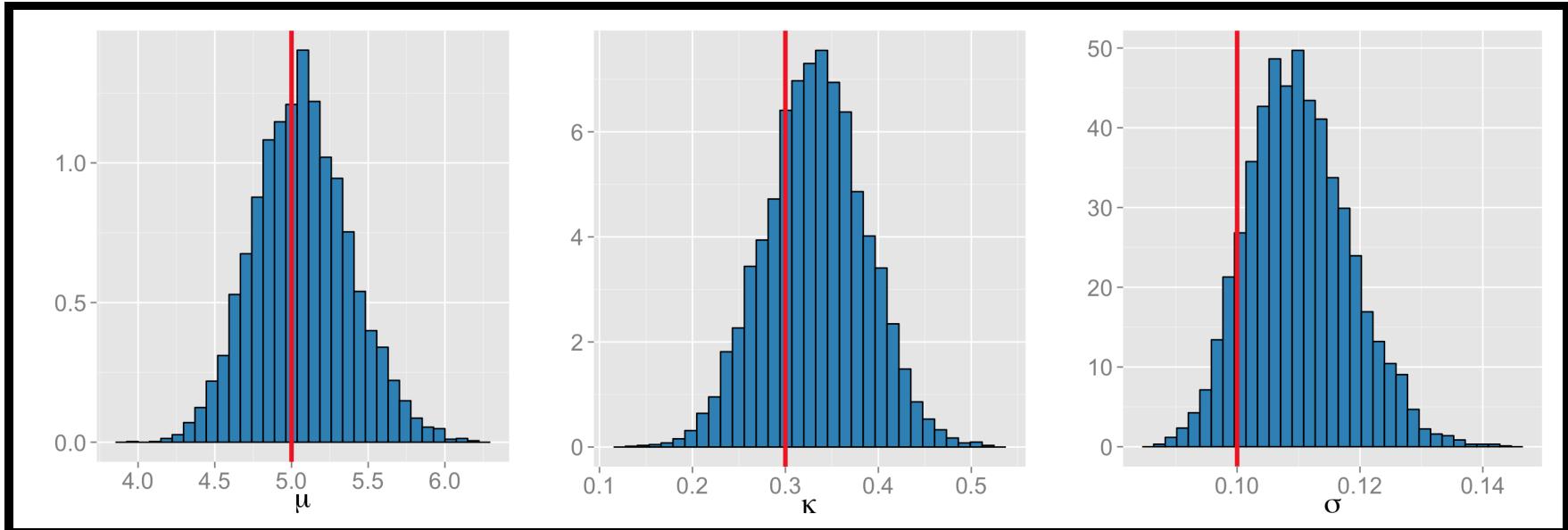
- Note that the tail of  $p(x_t | \mathbf{x}_{-t}, \mathbf{Y}, \Theta)$  is of the order  $\exp(-\mu e^{x_t})$ , which is very light
- So we can use independent Metropolis-Hastings with a normal instrumental density
  - The mean is chosen to be 0 since  $x(t)$  is an OU process with long-run average 0

# MCMC Algorithm

For  $k = 1, \dots, n$ , given  $(\mu^{(k)}, \kappa^{(k)}, \sigma^{(k)}, \mathbf{x}^{(k)})$ ,

1. Simulate  $\mu^{(k+1)}$  from Gamma posterior  $p(\mu | \kappa^{(k)}, \sigma^{(k)}, \mathbf{x}^{(k)})$
2. Simulate  $\kappa^{(k+1)}$  from normal posterior  $p(\kappa | \mu^{(k+1)}, \sigma^{(k)}, \mathbf{x}^{(k)})$
3. Simulate  $\sigma^{(k+1)^2}$  from inverse Gamma posterior  
 $p(\sigma^2 | \mu^{(k+1)}, \kappa^{(k+1)}, \mathbf{x}^{(k)})$
4. Use independent MH to iteratively simulate  $x_t^{(k+1)}$  from  
 $p(x_t | \mu^{(k+1)}, \kappa^{(k+1)}, \sigma^{(k+1)}, x_1^{(k+1)}, \dots, x_{t-1}^{(k+1)}, x_{t+1}^{(k)}, \dots, x_T^{(k)})$ ,  
for  $t = 1, \dots, T$ , with a normal instrumental density with  
mean 0

```
##      mu  kappa  sigma
## 5.0689 0.3321 0.1101
```



# Summary

- Bayesian inference + MCMC is powerful!
- However, fine tuning instrumental distributions and hyperparameters requires great effort!
- Do not blindly trust the results. If something is counter-intuitive, make sure find out why!