Statistical Inference

Lecture 02b

ANU - RSFAS

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Monte Carlo Integration

- Thus far we observe random variables $X_1, \ldots, X_N \sim f(x|\theta)$ and are concerned with using properties of $f(x|\theta)$ to describe the behavior of the random variables.
- Now we will generate random samples of X to learn about their behavior, as well as h(X).
- Monte Carlo integration:
 - Many quantities of statistical analyses can be expressed as the expectation of a function of a random variable E[h(X)].
 - Let $f(X|\theta)$ denote the density of X
 - Let μ denote the expectation of h(X).
 - Then when an iid sample X_1, \ldots, X_n is obtained from $f(X|\theta)$, we can approximate μ by a sample average:

$$\hat{\mu}_{MC} = \frac{1}{n} \sum_{i=1}^{n} h(X_i) \to \int h(x) f(x) dx = \mu$$

Monte Carlo Integration

• We can approximate σ^2 similarly:

$$\hat{\sigma}_{MC}^2 = \frac{1}{n-1} \sum_{i=1}^n (h(X_i) - \hat{\mu}_{MC})^2 \to \sigma^2$$

These results are based on the Law of Large Numbers.

Monte Carlo Integration

Example (Exponential lifetime):

 \bullet Suppose that a particular electrical component can be modeled with an exponential ($\beta=50)$ lifetime.

$$f(x|\beta) = \frac{1}{\beta} exp(-x/\beta)$$

• The manufacturer is interested in determining the probability that, out of c = 100 components, at least t = 35 of them will last h = 45 hours.

• We can first consider the analytical solution. The probability that a single component last at least h=45 is:

$$p_1 = \int_{45}^{\infty} \frac{1}{50} exp(-x/50) dx = 1/exp(45/50) \approx 0.4066$$

```
set.seed(1001)
n <- 20000
x <- rexp(n, 1/50)
x[1:5]</pre>
```

[1] 14.30061 34.86863 118.94469 42.38883 26.53421

mean(x)

[1] 50.22228

```
p1 <- length(x[x>=45])/n
p1
```

[1] 0.4082

mean(x>=45)

[1] 0.4082

$$p_2 = P(\text{at least } t = 35 \text{ components last at least } h = 45 \text{ hours})$$

$$= \sum_{t=35}^{100} \binom{100}{t} p_1^t (1-p_1)^{100-t}$$

[1] 0.895889

How about at least 90 out of 100 last at least 45 hours?

[1] 0

Full Monte Carlo Solution

- For j = 1, ..., n:
 - **1.** Generate $X_1, \ldots, X_{c=100} \stackrel{\text{iid}}{\sim} \text{exponential}(\beta = 50)$.
 - **2.** Set $Y_j = 1$ if at least t = 35 X_i s are $\geq h = 45$; otherwise set $Y_j = 0$.

Then, because $Y_j \sim \text{Bernoulli}(p_2)$ and $E[Y_j] = p_2$,

$$\frac{1}{n}\sum_{j=1}^{n}Y_{j}\to p_{2}\text{ as }n\to\infty$$

```
set.seed(1001)
n < -10000
y \leftarrow rep(0, n) \# storage
for(i in 1:n){
  x \leftarrow rexp(100, 1/50)
  if(length(x[x>=45])>=35){
  y[i] <- 1
mean(y)
```

[1] 0.8949

We can see that being able to generate random values from various probability distributions can be quite useful!

- There are a number of approaches to the generation of random variables.
- Let's start by considering the simplest approach, the probability integral transform.
- For this approach (and actually most every approach I can think of) we assume that we are able to generate:

$$U_1, \ldots U_m \stackrel{\text{iid}}{\sim} \text{uniform}(0,1)$$

Rice Section 2.3 Proposition C & D (Probability Integral Transform):

- Let X have a continuous cdf $F_X(x)$.
- Define the random variable $Y = F_X(x)$.
- Then Y is uniformly distributed on (0,1). $P(Y \le y) = y \quad 0 < y < 1$.

Proof:

$$P(Y \le y) = P(F_X(x) \le y)$$

$$= P(F_X^{-1}[F_X(x)] \le F_X^{-1}[y])$$

$$= P(X \le F_X^{-1}[y])$$

$$= F_X(F_X^{-1}[y]) = y$$

Note: If F_X is flat in a region then it may be that $F_X^{-1}[F_X(x)] \neq x$

- Let $x \in [x_1, x_2] \Rightarrow F_x^{-1}[F_X(x)] = x_1$ for any x in the interval.
- However, $P(X \le x) = P(X \le x_1)$.
- Generally we just define $F_X^{-1}(y) = \inf\{x | F(x) \ge y\}$

- Simply: $X = F_X^{-1}(U)$ has the distribution F_X .
- Consider $X \sim \text{exponential}(\beta = 2)$:

$$F_X(c) = \int_0^c \frac{1}{\beta} \exp(-x/\beta) dx = 1 - \exp(-c/\beta)$$

$$U = F_X(X) = 1 - \exp(-X/\beta)$$

$$U = F_X(X) = 1 - \exp(-X/\beta)$$

$$1 - U = \exp(-X/\beta)$$

$$\log(1 - U) = -X/\beta$$

$$-\beta \log(1 - U) = X = F_X^{-1}(U)$$

```
set.seed(1001)
u <- runif(10000, 0, 1)
x <- - 2*log(1-u)
mean(x)</pre>
```

[1] 1.989107

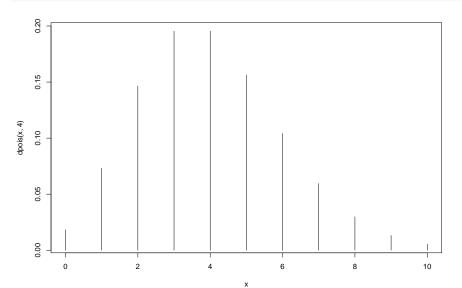
•
$$E[X] = \beta = 2$$
, $V(X) = \beta^2 = 4$

- Consider $X \sim \text{Poisson}(\lambda = 4)$ (density):
- P(X = 2) use 'd':

```
dpois(2, 4)
```

```
## [1] 0.1465251
```

```
x <- 0:10
plot(x, dpois(x, 4), type="h")</pre>
```



• $P(X \le 2)$ use 'p' (probability):

```
ppois(2, 4)
```

```
## [1] 0.2381033
```

• $P(X \le x^*) = 0.25$, to find x^* use 'q' (quantile):

[1] 3

• Remember the quantile must achieve the specified probability:

```
ppois(2, 4)
```

[1] 0.2381033

```
ppois(3, 4)
```

[1] 0.4334701

• So $x^* = 3$

• To generate random values use 'r'. Let's generate n=10 random values:

```
rpois(10, 4)
```

```
## [1] 2 6 7 3 1 7 1 5 4 4
```

• For an exponential (β) distribution we have:

$$Y_i = -\beta \log(1 - U_i)$$

As U is uniform (0,1) then we can simply sample by:

$$Y_i = -\beta log(U_i)$$

• Let's prove that if $U \sim \text{uniform}(0,1)$ then $Y = 1 - U \sim \text{uniform}(0,1)$.

- Based on the uniform-exponential relationship we can generate the following:
 - Sums of iid exponential random variables have a gamma distribution:

$$Y = -\beta \sum_{j=1}^{a} log(U_j) \sim \text{gamma}(a, \beta)$$

• If $\beta = 2$, then the distribution is a χ^2 random variable:

$$Y = -2\sum_{j=1}^{v} log(U_j) \sim \chi_{2v}^2$$

• The ratio of sums of exponentials is a beta distribution:

$$Y = \frac{\sum_{j=1}^{a} log(U_j)}{\sum_{j=1}^{a+b} log(U_j)} \sim \text{beta}(a, b)$$

- Let's generate some beta (a = 2, b = 5) random variables.
- If $X \sim \text{beta}(a = 2, b = 5)$, then

$$E[X] = \frac{a}{a+b} = \frac{2}{2+5} = 0.2857$$

$$V[X] = \frac{ab}{(a+b)^2(a+b+1)} = \frac{2(5)}{(2+5)^2(2+5+1)} = 0.02551$$

```
set.seed(1001)
n <- 10000
a < -2
b <- 5
y \leftarrow rep(0, n)
for(i in 1:n){
  u <- runif(a+b, 0, 1)
  y[i] <- sum(log(u[1:a]))/sum(log(u[1:(a+b)]))
mean(y)
```

```
var(y)
```

[1] 0.02523963

[1] 0.2853618

- Examine the following again:
 - If $\beta = 2$, then the distribution is a χ^2 random variable:

$$Y = -2\sum_{j=1}^{\nu} log(U_j) \sim \chi_{2\nu}^2$$

This suggests that we cannot simulate a χ_1^2 (or an odd number for v) random variable with this approach!

- If we could generate a normal(0,1) then we could generate a χ^2_1 .
- ullet There is no closed form solution to generate a single normal (0,1).
- Surprisingly through we can generate two independent normal (0,1) random variables!

- Example (Box-Muller Algorithm):
 - Generate U_1 , $U_2 \sim \text{uniform}(0,1)$.
 - Set:

$$R = \sqrt{-2log(U_1)}, \quad \theta = 2\pi U_2$$

• Then:

$$X = R\cos(\theta), \quad Y = R\sin(\theta)$$

- Then $X, Y \stackrel{\text{iid}}{\sim} \text{normal}(0, 1)$
- If we want two samples from a χ_1^2 all we have to do is:

$$X^2, Y^2$$

• So far we have considered continuous distributions.

$$F_Y^{-1}(u) = y \leftrightarrow u = \int_{-\infty}^{y} f_Y(t) dt$$

- Now let's sample from discrete distributions.
- If Y is a discrete random variable taking on values:

$$y_1 < y_2 < \cdots < y_k$$

then we can write:

$$P[F_Y(y_i) < U \le F_Y(y_{i+1})] = F_Y(y_{i+1}) - F_Y(y_i)$$

= $P(Y = y_{i+1})$

Using this idea we can easily discrete random variables. To generate $Y_i \sim f_Y(y)$:

- **1.** Generate $U \sim \text{uniform}(0, 1)$.
- **2.** If $F_Y(y) < U \le F_Y(y_{i+1})$, $set Y = y_{i+1}$.

Define $y_0 = -\infty$ and $F_Y(y_0) = 0$.

- Example (Binomial random variable generation)
- Let's generate random variables from $Y \sim \text{binomial}(n = 4, p = 5/8)$.
- **1.** Generate $U \sim \text{uniform}(0, 1)$.
- **2.** Determine *Y*:

$$Y = \left\{ \begin{array}{ll} 0 & \text{if } 0 < U \leq 0.020 \\ 1 & \text{if } 0.020 < U \leq 0.152 \\ 2 & \text{if } 0.152 < U \leq 0.481 \\ 3 & \text{if } 0.481 < U \leq 0.847 \\ 4 & \text{if } 0.847 < U \leq 1 \end{array} \right.$$

```
set.seed(2001)
n <- 10000
u \leftarrow runif(n, 0, 1)
y \leftarrow qbinom(u, 4, 5/8)
mean(y)
```

```
## [1] 2.4971
```

```
var(y)
```

[1] 0.9496866
$$E[Y] = np = 4(5/8) = 2.5, \quad V[Y] = np(1-p) = 4(5/8)(1-5/8) = 0.9375$$

Indirect Sampling Methods

- Thus we we considered direct sampling methods (generate X then apply a function to get Y directly), now we will consider indirect methods.
- Indirect methods are useful when we don't have a nice analytical solution to the inverse of the function of interest.

Theorem (The Accept/Reject Algorithm):

• Let $Y \sim f_Y(y)$ and $V \sim f_V(v)$, where densities have common support and

$$M = \sup_{y} \frac{f_{Y}(y)}{f_{V}(y)} < \infty$$

- ullet Suppose we want to sample from Y and are able to sample from V.
- **1.** Generate $U \sim \text{uniform}(0,1)$ and $V \sim f_V$, independently.
- **2.** If $U < \frac{1}{M} \frac{f_Y(V)}{f_V(V)}$, set Y = V; otherwise return to (1).

Note: envelope = $M f_V(v) \ge f_Y(v)$.

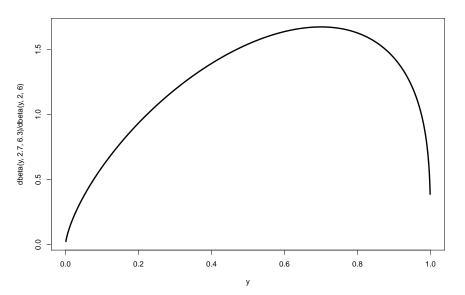
- Example 5.6.9:
 - We know how to generate $V \sim \text{beta}(2,6)$, see slide 3.
 - Now let's generate $Y \sim \text{beta}(2.7, 6.3)$. The previous method will not work!
 - Lets first figure out *M*:

$$M = \sup_{y} \frac{f_{Y}(y)}{f_{V}(y)}$$

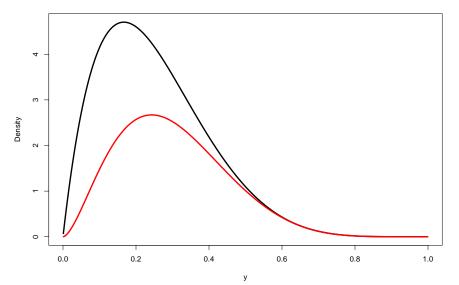
```
y <- seq(0.001, 0.999, by=0.001)
M <- max(dbeta(y, 2.7, 6.3)/dbeta(y, 2, 6))
M
```

```
## [1] 1.671808
```

plot(y, dbeta(y, 2.7, 6.3)/dbeta(y, 2, 6), type="1", lwd=3)



plot(y, M*dbeta(y, 2, 6), type="1", lwd=3, ylab="Density")
lines(y, dbeta(y, 2.7, 6.3), lwd=3, col="red")



```
set.seed(1001)
n <- 10000
y <- NULL
for(i in 1:n){
u \leftarrow runif(1, 0, 1)
v \leftarrow rbeta(1, 2, 6)
if(u < (1/M)*(dbeta(v, 2.7, 6.3)/dbeta(v, 2, 6))){}
y.i <- v
 y \leftarrow c(y, y.i)
}}
length(y)
```

```
## [1] 6039
```

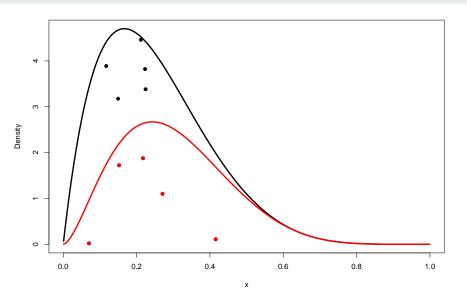
First 10 Draws

points(v.out[v.out==1], m.v.u[v.out==1], pch=19, col="red")

set.seed(1001) n <- 10

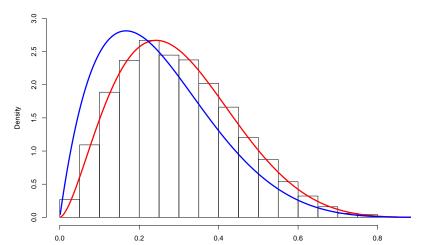
```
m.v.u \leftarrow rep(0, 10)
v.out <- rep(0, 10)
v.out <- rep(0,10)
for(i in 1:n){
u \leftarrow runif(1, 0, 1)
v \leftarrow rbeta(1, 2, 6)
v.out[i] <- v
m.v.u[i] <- M*dbeta(v. 2, 6)*u
if(u < (1/M)*(dbeta(v, 2.7, 6.3)/dbeta(v, 2, 6))){}
 y.out[i] <- 1
  }}
x \leftarrow seq(0.001, 0.999, by=0.001)
plot(x, M*dbeta(x, 2, 6), type="1", lwd=3, ylab="Density")
lines(x, dbeta(x, 2.7, 6.3), lwd=3, col="red")
points(v.out, m.v.u, pch=19)
```

First 10 Draws



```
hist(y, prob=TRUE, ylim=c(0,3))
x <- seq(0.001, 0.999, by=0.001)
lines(x, dbeta(x, 2.7, 6.3), lwd=3, col="red")
lines(x, dbeta(x, 2, 6), lwd=3, col="blue")
```

Histogram of y



Proof:

$$\begin{split} P(Y \leq y) &= P\left(V \leq y | U < \frac{1}{M} \frac{f_Y(V)}{f_V(V)}\right) \\ &= P\left(V \leq y | U < \frac{1}{M} \frac{f_Y(V)}{f_V(V)}\right) \\ &= \frac{P\left(V \leq y \text{ and } U < \frac{1}{M} \frac{f_Y(V)}{f_V(V)}\right)}{P\left(U < \frac{1}{M} \frac{f_Y(V)}{f_V(V)}\right)} \\ &= \frac{\int_{-\infty}^{y} \int_{0}^{\frac{1}{M} \frac{f_Y(V)}{f_V(V)}} f_U(u) f_V(v) du dv}{\int_{-\infty}^{\infty} \int_{0}^{\frac{1}{M} \frac{f_Y(V)}{f_V(V)}} 1 f_V(v) du dv} \\ &= \frac{\int_{-\infty}^{y} \frac{1}{M} f_Y(v) dv}{\frac{1}{M}} = \int_{-\infty}^{y} f_Y(v) dv \end{split}$$

• What can we say about M?

$$P(\text{stop}) = P\left(U < \frac{1}{M} \frac{f_{Y}(V)}{f_{V}(V)}\right)$$

$$= \int_{-\infty}^{\infty} \int_{0}^{1} \frac{f_{Y}(v)}{f_{V}(v)} f_{U}(u) f_{V}(v) du dv = \int_{-\infty}^{\infty} \int_{0}^{1} \frac{f_{Y}(v)}{f_{V}(v)} 1 du f_{V}(v) dv$$

$$= \int_{-\infty}^{\infty} \frac{1}{M} \frac{f_{Y}(v)}{f_{V}(v)} f_{V}(v) dv$$

$$= \int_{-\infty}^{\infty} \frac{1}{M} f_{Y}(v) dv$$

$$= \frac{1}{M} \int_{-\infty}^{\infty} f_{Y}(v) dv$$

$$= \frac{1}{M} \times 1 = \frac{1}{M}$$

- We are considering the number of trials till a success (a geometric distribution). If $W \sim \operatorname{geometric}(\theta)$ then $E[W] = 1/\theta$.
 - The probability of success is:

$$p = 1/M$$

The expected number of draws till a success:

$$1/p = M$$

• In our example we found M = 1.672. In the end we had 6,039 successes.

$$6,039 \times 1.672 = 10,097.21 \approx n = 10,000$$

- Various specialized versions of this technique exist to solve particular problems (See Givens and Hoeting):
 - Squeezed Rejection Sampling (cases where evaluating $f_Y(y)$ is computationally expensive)
 - Adaptive Rejection Sampling (adaptively generates a suitable envelope).

- For the standard accept/reject algorithm we need a good envelope. For some distributions that may be difficult.
- When a good envelope is not available Markov chain Monte Carlo (MCMC) can aid in sampling for a desired target distribution:
 - Metropolis algorithm
 - Metropolis-Hastings algorithm
 - Gibbs sampling
 - ...

Metropolis-Hastings Algorithm

- Let $Y \sim f_Y(y)$ and $Y^* \sim f_V(v)$, where f_Y and f_V have common support. Then to generate $Y \sim f_Y$:
 - 1. Set $Z_0 = c$ any starting value. This could be by drawing a Y^* from $f_V(v)$.
 - **2.** For $i = 1, \ldots$:
 - **2.1** Generate $Y_i^* \sim f_V$ and $U_i \sim \text{uniform}(0,1)$ and calculate:

$$ho_i = \min \left\{ \underbrace{\frac{f_{V}(Y_i^*)}{f_{V}(Z_{i-1})}}_{ ext{ratio of target density}} imes \underbrace{\frac{f_{V}(Z_{i-1})}{f_{V}(Y_i^*)}}_{ ext{ratio of proposal density}}, 1
ight\}$$

2.2 Set

$$Z_i = \begin{cases} Y_i^* & \text{if } U_i \le \rho_i \\ Z_{i-1} & \text{if } U_i > \rho_i \end{cases}$$

As $i \to \infty$, Z_i converges to Y in distribution.

- If the proposal distirbution is symmetric, $f_V(Z_{i-1}|Y_i^*) = f_V(Y_i^*|Z_{i-1})$, then we have the Metropolis algorithm:
 - 1. Set $Z_0 = c$ any starting value. This could be by drawing a Y^* from $f_V(v)$.
 - **2.** For $i = 1, \ldots$:
 - **2.1** Generate $Y_i^* \sim f_V$ and $U_i \sim \mathrm{uniform}(0,1)$ and calculate:

$$\rho_i = \min \left\{ \frac{f_Y(Y_i^*)}{f_Y(Z_{i-1})}, 1 \right\}$$

2.2 Set

$$Z_i = \left\{ \begin{array}{ll} Y_i^* & \text{if } U_i \le \rho_i \\ Z_{i-1} & \text{if } U_i > \rho_i \end{array} \right.$$

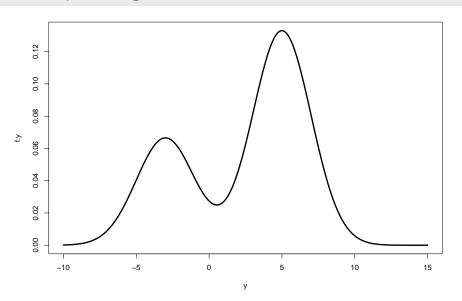
As $i \to \infty$, Z_i converges to Y in distribution.

- Intuition:
 - If $\frac{f_Y(Y_i^*)}{f_Y(Z_{i-1})} > 1$, then accept Y^* as it has a higher 'probability' than Z_{i-1} .
 - If $r = \frac{f_Y(Y_i^*)}{f_Y(Z_{i-1})} \le 1$, then accept Y^* at the rate r.
- Common symmetric proposal distributions:
 - $f_V(Y_i^*|Z_{i-1}) = \text{uniform}(Z_{i-1} \delta, Z_{i-1} + \delta)$
 - $f_V(Y_i^*|Z_{i-1}) = \text{normal}(\mu = Z_{i-1}, \sigma)$
 - \bullet $\,\delta$ and $\,\sigma$ are called tuning parameters and control the size of the 'jump'.

 Let's use the Metropolis algorithm to generate values from the following mixture distribution:

$$f_Y(y) = \frac{1}{3} \operatorname{normal}(\mu = -3, \sigma = 2) + \frac{2}{3} \operatorname{normal}(\mu = 5, \sigma = 2)$$

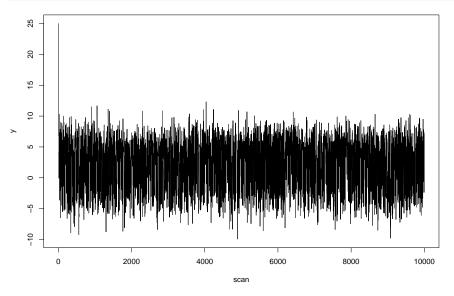
```
y <- seq(-10, 15, by=0.01)
f.y <- (1/3)*dnorm(y,-3, 2) + (2/3)*dnorm(y, 5, 2)
plot(y, f.y, type="l", lwd=3)
```



Metropolis Algorithm $\delta = 10$

```
set.seed(1001)
S <- 10000
out <- rep(0, S)
acc <- 0
## density
f.y <- function(y){
  out <- (1/3)*dnorm(y,-3, 2) + (2/3)*dnorm(y, 5, 2)
  return(out)
## starting value
v <- 25
out[1] <- y
## tuning parameter
delta <- 10
## MCMC
for(i in 2:S){
  y.star <- runif(1, y-delta, y+delta)
  r \leftarrow f.y(y.star)/f.y(y)
  rho \leftarrow min(r,1)
  if(runif(1) <= rho){
    y <- y.star
    acc <- acc + 1
  out[i] <- y
```

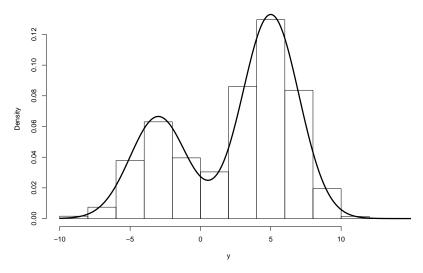
plot(out, type="l", ylab="y", xlab="scan")



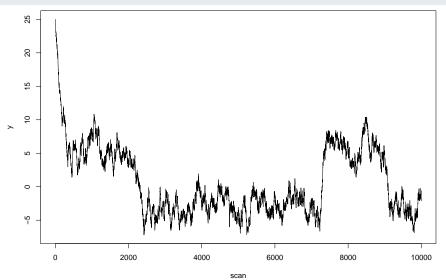
The acceptance rate was 0.5099.

• let's remove the first 100 values for burn-in.

Samples from the Mixture of Normals

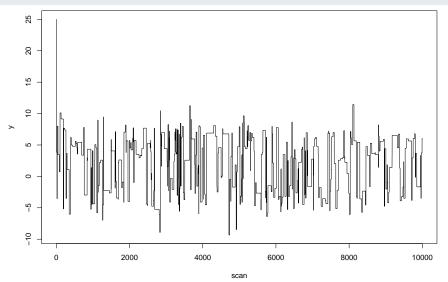


Metropolis Algorithm - Small $\delta=0.5$



The acceptance rate was 0.9566.

Metropolis Algorithm - Large $\delta=150$



The acceptance rate was 0.0372.

MCMC

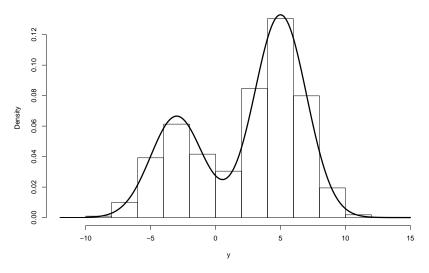
 As you might expect there are numerous variations on the Metropolis-Hastings approach in order to efficiently sample for the target distribution. See Givens and Hoeting for more information.

- Based on what we know we can consider a direct approach to the simulation of the mixture of normals:
 - **1.** Generate $X \sim \text{Bernoulli}(p = 1/3)$.
 - 2. If X=1 generate $Z\sim \mathrm{normal}(\mu=-3,\sigma=2)$. If X=0 generate $Z\sim \mathrm{normal}(\mu=5,\sigma=2)$.

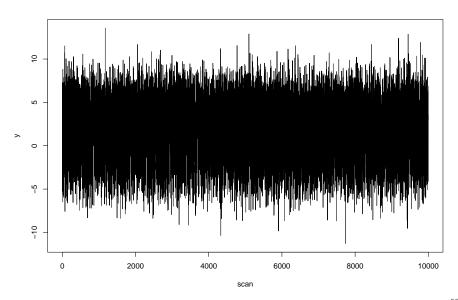
```
set.seed(1001)
n <- 10000
out <- rep(0, n)
x <- rbinom(n, 1, 1/3)

out[x==1] <- rnorm(length(out[x==1]), -3, 2)
out[x==0] <- rnorm(length(out[x==0]), 5, 2)</pre>
```

Samples from the Mixture of Normals



plot(out, type="1", ylab="y", xlab="scan")



Moving Forward

- In Chapter 6 we will cover:
 - Distirbutions derived from normal distributions