Metropolis-Hastings

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General Metropolis-Hastings

Given a target density f, we build a Markov kernel K with stationary distribution f and then generate a Markov chain X_t using this kernel so that the limiting distribution of X_t is f and integrals can be approximated according to the Ergodic Theorem.

The **Metropolis-Hastings algorithm** is a general purpose MCMC method for approximating a f. Given the target density f and a conditional density $q(y|x)$ that is easy to simulate from. In addition, q can be almost arbitrary in that the only theoretical requirements are that the ration $\frac{f(y)}{q(y|x)}$ is known up to a constant *independent* of x and that $q(\cdot|x)$ has enough dispertion to lead to an exploration of the entire support of f

We can rely on the feature of Metropolis-Hatings algorithm that for every given q, we can then construct a Metropolis-Hastings kernel such that f is its stationary distribution.

The Metropolis-Hastings algorithm as described Robert & Casella goes as follows Given $x^{(t)}$

1. Generate $Y_t \sim q(y|x_t)$

2. Take
$$
X_{t+1} = \begin{cases} Y_t & \text{with probability } \rho(x^{(t)}, Y_t) \\ x^{(t)} & \text{with probability } 1 - \rho(x^{(t)}, Y_t) \end{cases}
$$

where
$$
\rho(x^{(t)}, Y_t) = \min\{\frac{f(Y_t)}{f(x^{(t)})} \frac{q(x^{(t)}|Y_t)}{q(Y_t|x^{(t)})}, 1\}
$$

In simpler terms, as we want to generate $X \sim f$, we first take an initial value $x^{(0)}$ (which can almost be any artibrary value in the support of f).

1. We generate a value $Y_0 \sim q(y|x^{(0)})$.

2. We calculate $\rho(x^{(t)}, Y_t)$

3. Generate a random value $U \sim Unif(0, 1)$

4. If $U < \rho(x^{(t)}, Y_t)$, then we accept $X^{(1)} = Y_t$; else we take $X^{(1)} = X^{(0)}$

5. Repeat steps 1-4 until you've satisfied the number of samples needed

Example 6.1: Beta(2.7, 6.3)

As of now, we've covered multiple ways of generating random samples from a target density. Let us compare the accept-reject algorithm once more with the Metropolis-Hastings algorithm. Generate N samples from $Beta(2.7, 6.3)$

In order to use the accept-reject algorithm, we need a candidate distribution to sample from. Below are a set of potential candidate distributions.

```
## potential instumential distributions
curve(expr = dbeta(x, 2.7, 6.3), from = 0, to = 2)
curve(expr = dbeta(x, 3, 6), from = 0, to = 2, add = TRUE, col = 2, lty = 2)
curve(expr = dexp(x, rate = 3), from = 0, to = 2, add = TRUE, col = 3, lty = 2)
#curve(expr = dnorm(x, mean = 1, sd = 1), from = 0, to = 2, add = TRUE, col = 4, lty = 2)
curve(expr = dnorm(x, mean = 0.25, 0.25), from = -2, to = 2, add = TRUE, col = 4, lty = 2)
```
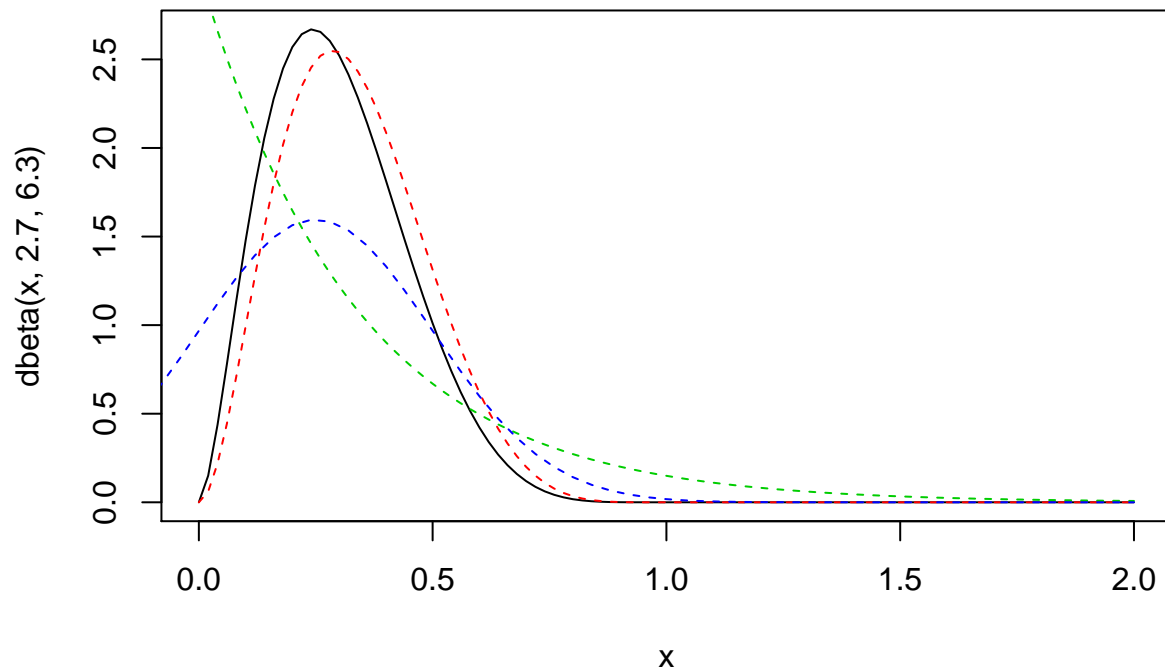


```
fg = function(x){
  1.5*dbeta(x, 2.7, 6.3)/dexp(x, rate = 1)
}

curve(expr = fg, from = 0, to = 2)
curve(expr = dbeta(x, 2.7, 6.3), from = 0, to = 2, add = TRUE, lty = 3)
```
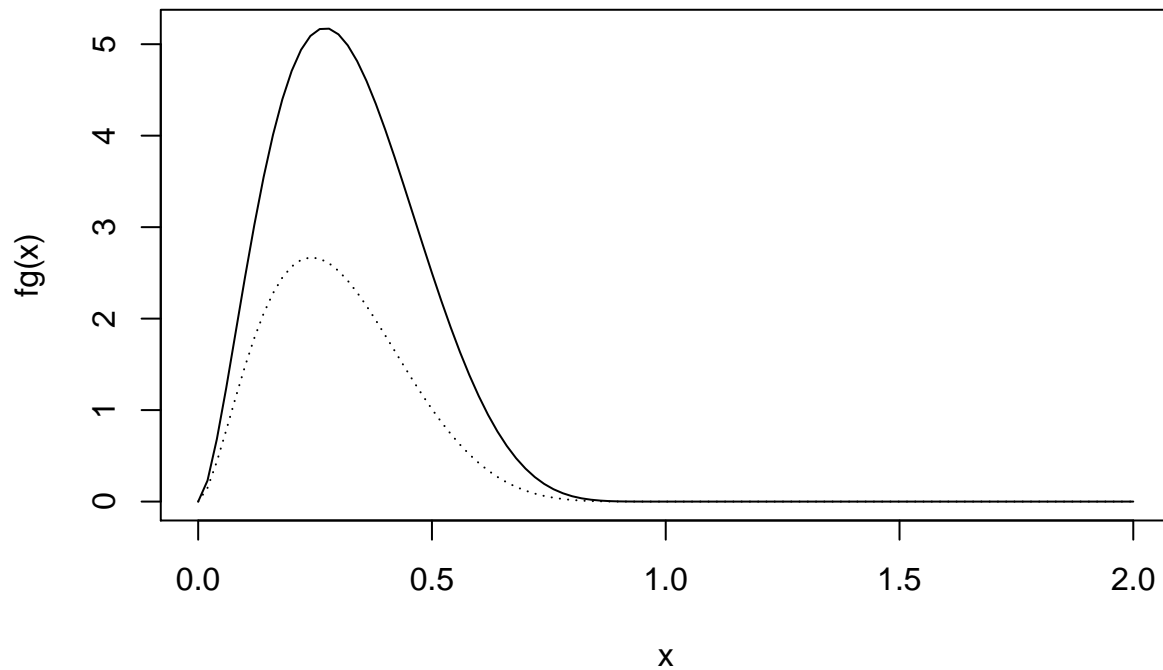
We will use $Exp(3)$ as our candidate distribution, g.

```r
N = 10000

## For accept-reject, we need to find a value for M
## we can use `optimize` to find the maximum of our target density
maximum  = optimize(f = function(x){ dbeta(x, 2.7, 6.3) },
                    interval = c(0, 2), maximum = TRUE ) ## obtain maximum

## M here is basically random guess
M = maximum$objective  ## something smaller like 1.5 works too!
curve(expr = dbeta(x, 2.7, 6.3),
      from = 0, to = 2, col = "blue",
      main = "Beta(2.7, 6.3)", xlab = "X", ylab = "Density")
abline(h = M, lty = 2, lwd = 2, col = "red")
```

Beta(2.7, 6.3)
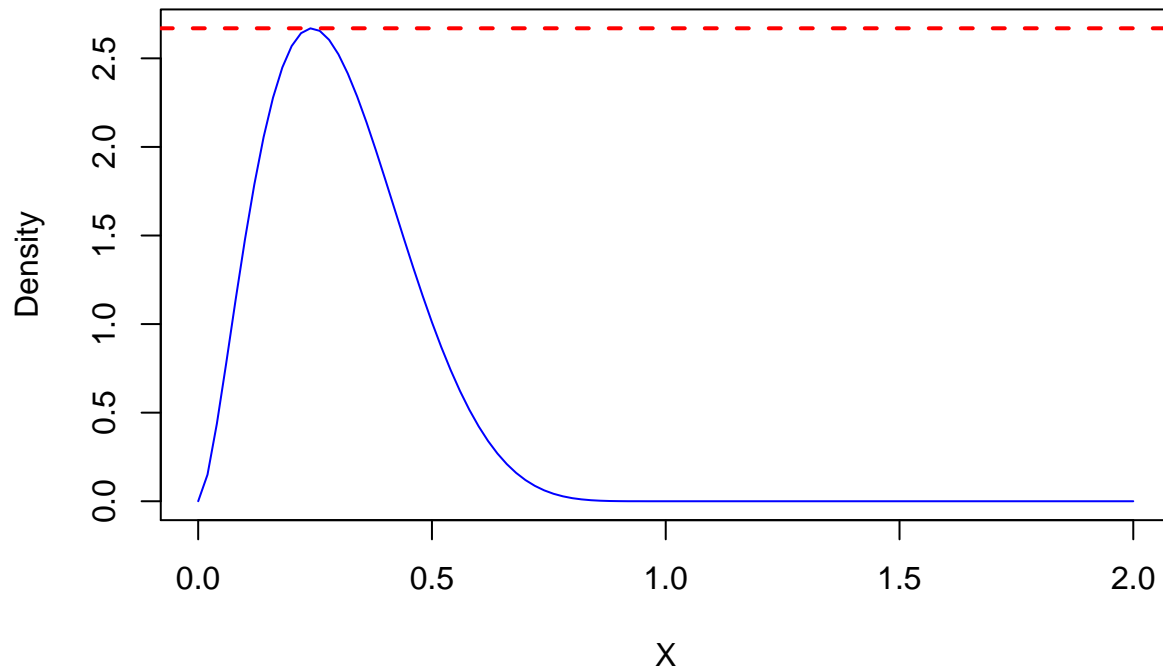

```r
f = function(x){
  dbeta(x, 2.7, 6.3)
}

g = function(x){
  #dnorm(x, mean = maximum$maximum, sd = 0.25)
  dexp(x, rate = 1)
}


#N = 100000
X = numeric(N)
i = 0
while(i < N){
  #Y = abs(rnorm(n = 1, mean = maximum$maximum, sd = 0.25))
  Y = rexp(n = 1, rate = 1)
  U = runif(1)
  if(U*M <= f(Y)/g(Y)){
    i = i + 1
    X[i] = Y
  }
}


print("sample mean from direct samples")

## [1] "sample mean from direct samples"
```

```r
mean(rbeta(n = 1000, shape1 = 2.7, shape2 = 6.3))
```
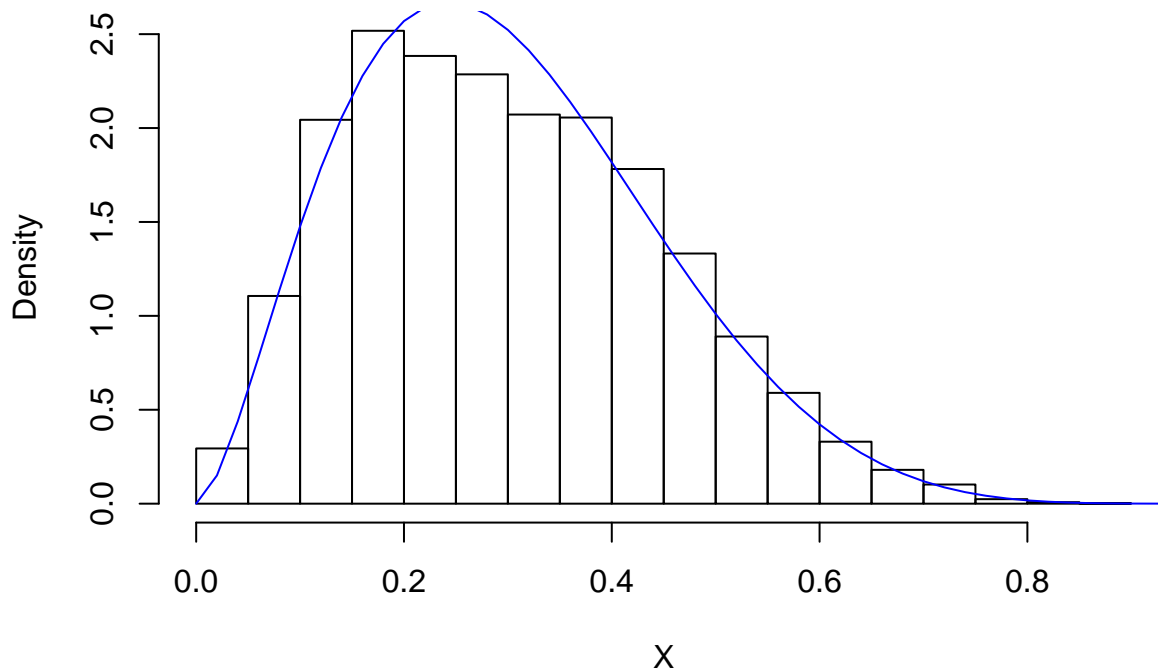
```
## [1] 0.2992948
```

```r
print("sample mean from Accept-Reject samples")
```

```
## [1] "sample mean from Accept-Reject samples"
```

```r
mean(X)
```

```
## [1] 0.3011396
```

```r
## see how samples from chain compare to Beta(2.7, 6.3) density
hist(X, main = "Histogram of MCMC samples", prob = TRUE)
curve(expr = dbeta(x, 2.7, 6.3),
      from = 0, to = 2, add = TRUE, col = "blue")
```

Histogram of MCMC samples

Below is the Metropolis-Hastings implementation for this problem.

```r
## Metropolis Hastings
## now compare results with Beta(2.7, 6.3)

N = 10000
X = numeric(N)
X[1] = rbeta(n = 1, shape1 = 2.7, shape2 = 6.3) ## initial value
for(i in 1:N){
  Y = rexp(n = 1, rate = X[i])
  rho = (dbeta(x = Y, 2.7, 6.3) * dexp(x = X[i], rate = Y)) /
    (dbeta(x = X[i], 2.7, 6.3) * dexp(x = Y, rate = X[i]))

  if(runif(1) < rho){
    X[i+1] = Y
```

```
  } else{
    X[i+1] = X[i]
  }

}

print("sample mean from direct samples")

## [1] "sample mean from direct samples"
mean(rbeta(n = 1000, shape1 = 2.7, shape2 = 6.3))

## [1] 0.3028107
print("sample mean from M-H samples")

## [1] "sample mean from M-H samples"
mean(X)

## [1] 0.2978096
## see chain transitions
plot(X, type = "o", main = "MCMC samples",
     xlim = c(500,1000),
     xlab = "iterations", ylab = "X (samples obtained)")
```
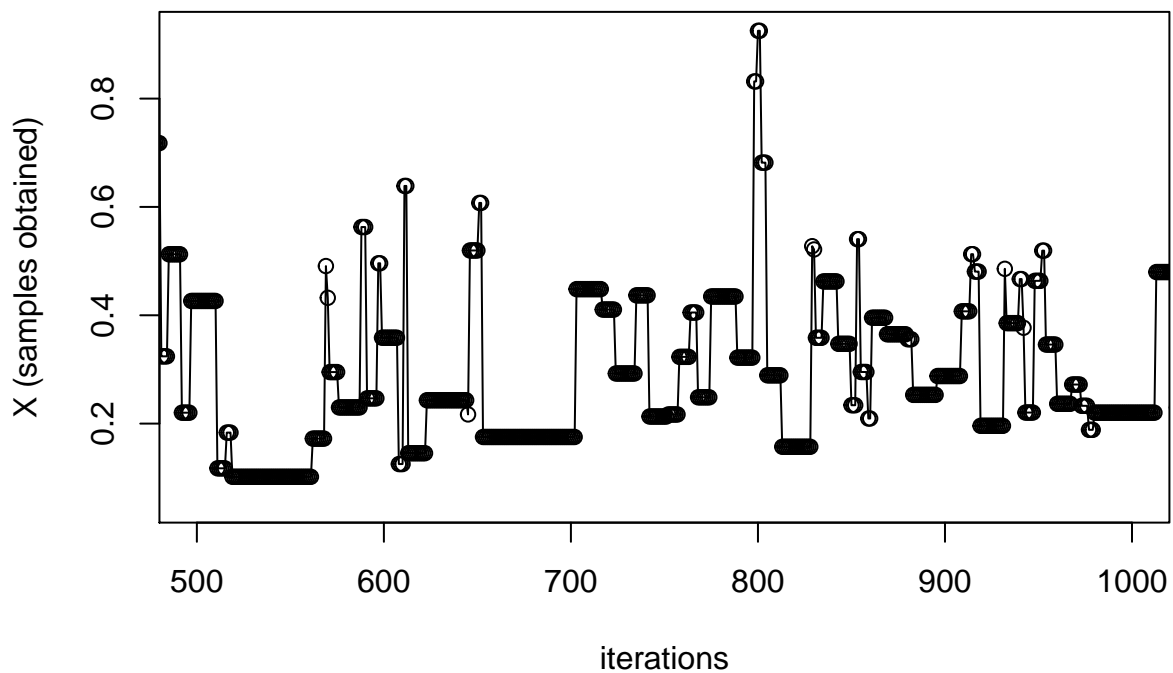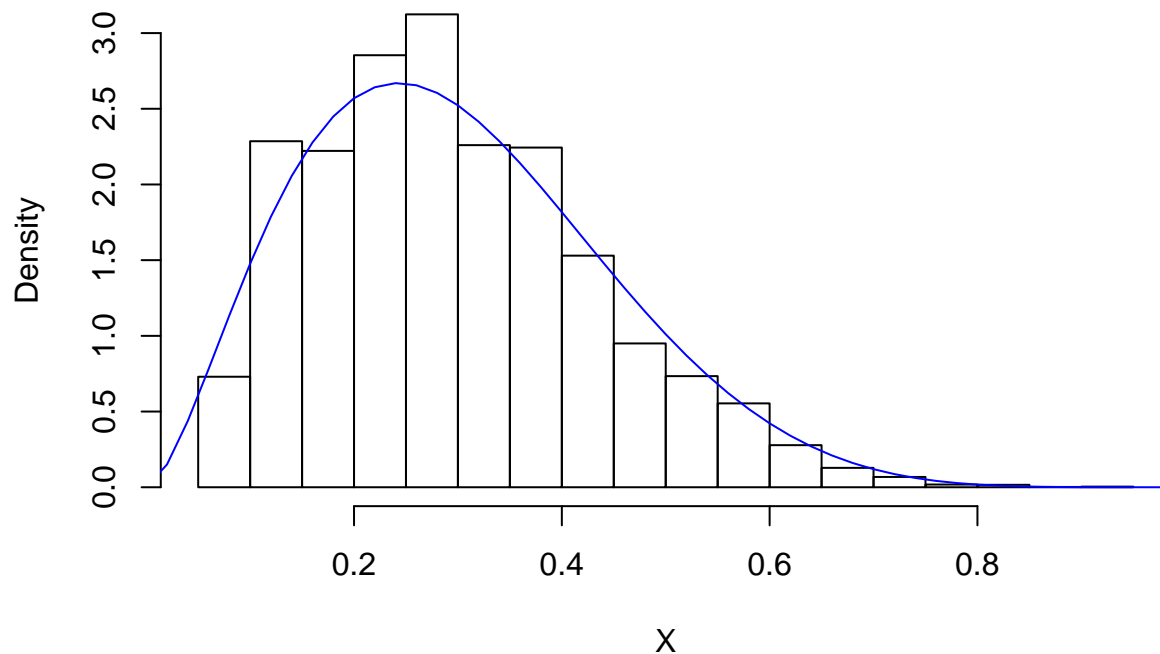
MCMC samples


```
## see how samples from chain compare to Beta(2.7, 6.3) density
hist(X, main = "Histogram of MCMC samples", prob = TRUE)
curve(expr = dbeta(x, 2.7, 6.3),
      from = 0, to = 2, add = TRUE, col = "blue")
```

Histogram of MCMC samples

Here is a varition of the M-H algorithm used previously, except we do not let the candidate distribution depend on previous values of the chain. The candidate distribution depends only on present values of the chain, in effect $q(y|x) = q(y)$.

```
## Metropolis Hastings
## now compare results with Beta(2.7, 6.3)

N = 10000
X = numeric(N)
X[1] = rbeta(n = 1, shape1 = 2.7, shape2 = 6.3)
for(i in 1:N){
  Y = rexp(n = 1, rate = 1)
  rho = (dbeta(x = Y, 2.7, 6.3) * dexp(x = X[i], rate = 1)) /
    (dbeta(x = X[i], 2.7, 6.3) * dexp(x = Y, rate = 1))

  if(runif(1) < rho){
    X[i+1] = Y
  } else{
    X[i+1] = X[i]
  }

}


print("sample mean from direct samples")

## [1] "sample mean from direct samples"
```

```r
mean(rbeta(n = 1000, shape1 = 2.7, shape2 = 6.3))
```

```
## [1] 0.3010068
```

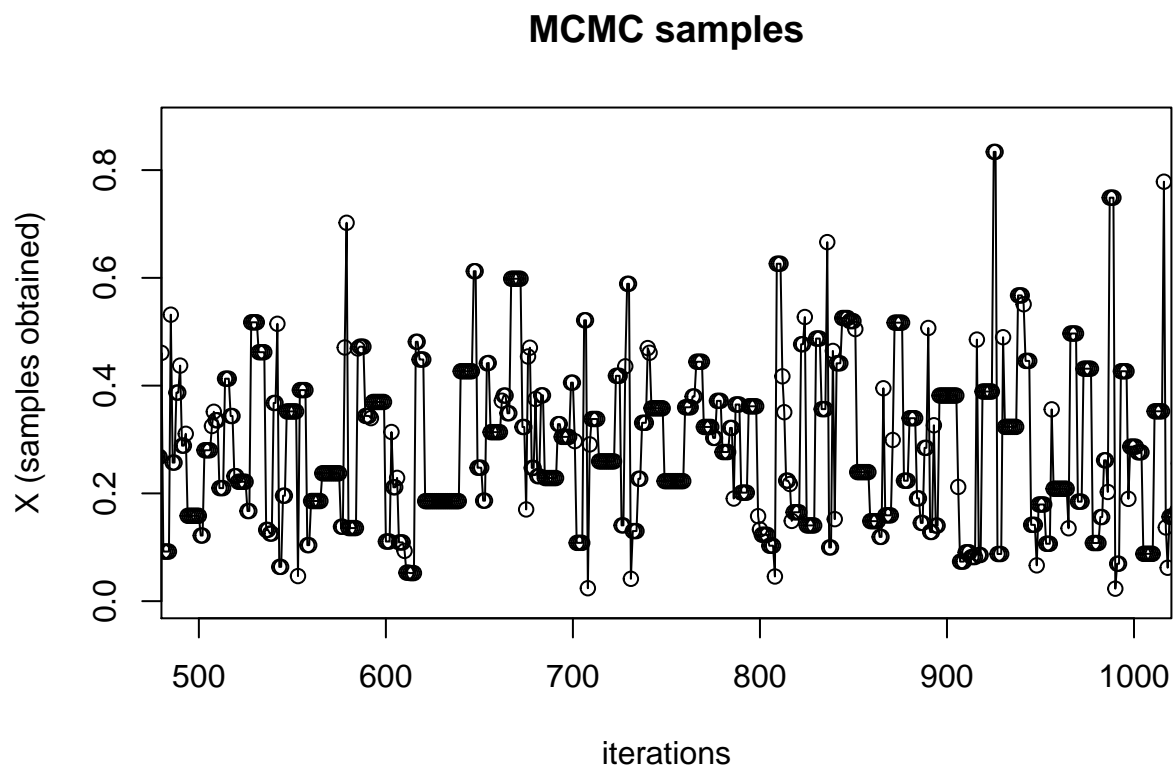```r
print("sample mean from M-H samples")
```

```
## [1] "sample mean from M-H samples"
```

```r
mean(X)
```

```
## [1] 0.3068487
```

```r
## see chain transitions
plot(X, type = "o", main = "MCMC samples",
     xlim = c(500,1000),
     xlab = "iterations", ylab = "X (samples obtained)")
```
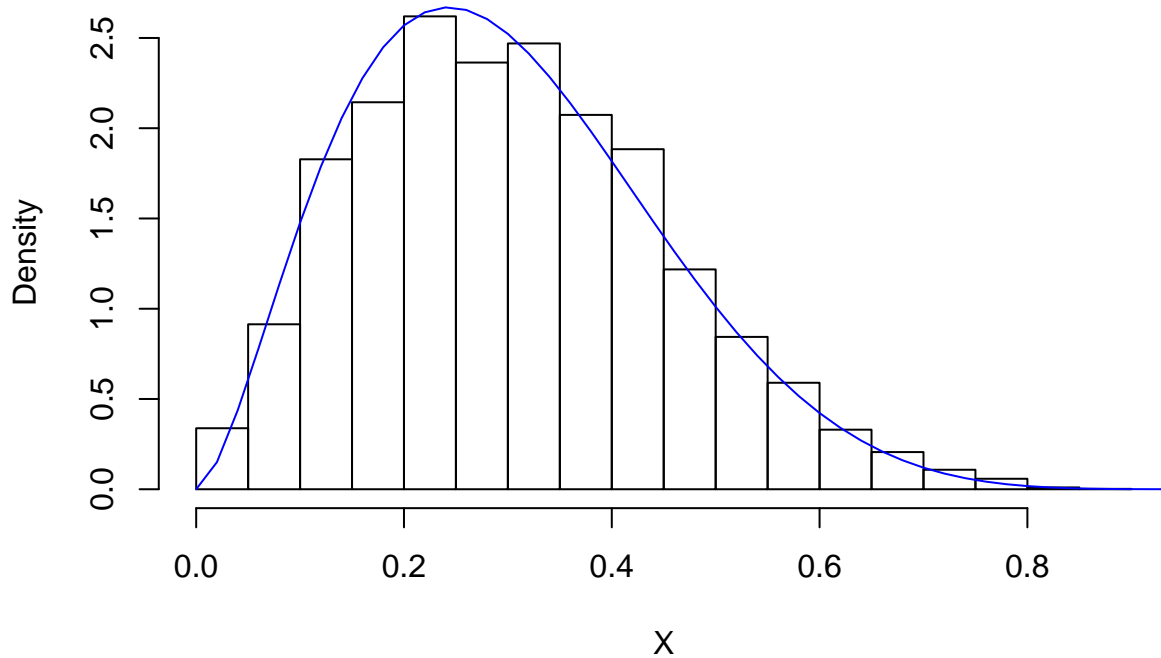


```r
## see how samples from chain compare to Beta(2.7, 6.3) density
hist(X, main = "Histogram of MCMC samples", prob = TRUE)
curve(expr = dbeta(x, 2.7, 6.3),
      from = 0, to = 2, add = TRUE, col = "blue")
```

Histogram of MCMC samples

This version of the M-H algorithm is known as the **Independent Metropolis-Hastings**. This method appears a generalization of the accept-reject algorithm in the sense that the instrumental distribution is the same density g as in the accept-reject algorithm. Thus, the proposed values Y_i are the same, if not the accepted ones.

The **Independent Metropolis-Hastings algorithm** as described Robert & Casella goes as follows Given $x^{(t)}$

1. Generate $Y_t \sim g(y)$

2. Take

$$X_{t+1} = \begin{cases} Y_t & \text{with probability } \ \rho(x^{(t)}, Y_t) \\ x^{(t)} & \text{with probability } \ 1 - \rho(x^{(t)}, Y_t) \end{cases}$$

where

$$\rho(x^{(t)}, Y_t) = \min\{\frac{f(Y_t)}{f(x^{(t)})} \frac{g(x^{(t)})}{g(Y_t)}, 1\}$$

In simpler terms, as we want to generate $X \sim f$, we first take an initial value $x^{(0)}$ (which can almost be any artibrary value in the support of f).

1. We generate a value $Y_0 \sim q(y|x^{(0)})$.

2. We calculate $\rho(x^{(t)}, Y_t)$

3. Generate a random value $U \sim Unif(0, 1)$

4. If $U < \rho(x^{(t)}, Y_t)$, then we accept $X^{(1)} = Y_t$; else we take $X^{(1)} = X^{(0)}$

5. Repeat steps 1-4 until you've satisfied the number of samples needed

Example: Gamma(4.3, 6.2)

Here we will compare again the Accept-Reject algorithm against the Metropolis-Hastings. Generate N random variables $X \sim Gamma(4.3, 6.2)$.

```
N = 10000

## For accept-reject, we need to find a value for M
## we can use `optimize` to find the maximum of our target density
maximum  = optimize(f = function(x){ dgamma(x = x, shape = 4.3, rate = 6.2)},
                    interval = c(0, 2), maximum = TRUE ) ## obtain maximum

M = maximum$objective
curve(expr = dgamma(x = x, shape = 4.3, rate = 6.2),
      from = 0, to = 2, col = "blue",
      main = "Gamma(4.3, 6.2", xlab = "X", ylab = "Density")
abline(h = M, lty = 3, lwd = 2, col = "red")
```


Gamma(4.3, 6.2
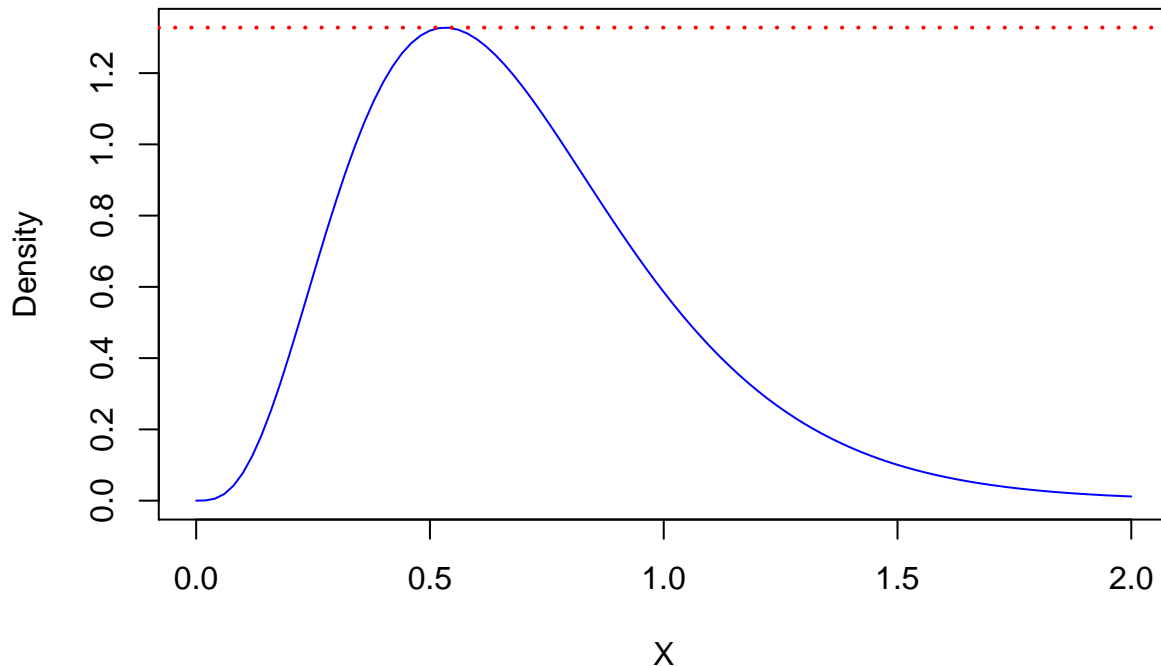
```
f = function(x){
  dgamma(x = x, shape = 4.3, rate = 6.2)
}

g = function(x){
  dgamma(x = x, shape = 4, rate = 7)
}


#N = 10
X = numeric(N)
i = 0
```
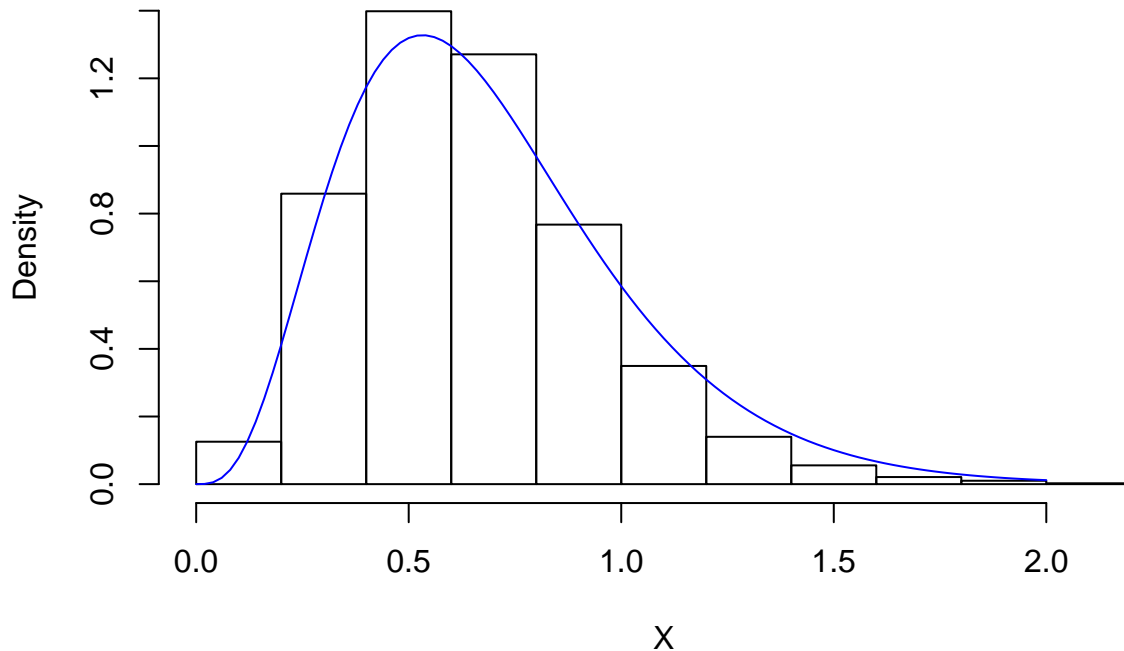
```
while(i < N){
  Y = rgamma(n = 1, shape = 4, rate = 7)
  U = runif(1)
  if(U*M <= f(Y)/g(Y)){
    i = i + 1
    X[i] = Y
  }
}

## see how samples from chain compare to Gamma density
hist(X, main = "Histogram of MCMC samples", prob = TRUE)
curve(expr = dgamma(x = x, shape = 4.3, rate = 6.2),
      from = 0, to = 2, add = TRUE, col = "blue")
```

Histogram of MCMC samples


```
## Metropolis Hastings

N = 10000
X = numeric(N)
X[1] = rgamma(n = 1, shape = 4.3, rate = 6.2)
for(i in 1:N){
  Y = rgamma(n = 1, shape = 4, rate = 7)
  rho = (dgamma(x = Y, shape = 4.3, rate = 6.2) * dgamma(x = X[i], shape = 4, rate = 7)) /
    (dgamma(x = X[i], shape = 4.3, rate = 6.2) * dgamma(x = Y, shape = 4, rate = 7))
  #X[i+1] = X[i] + (Y - X[i])*(runif(1) < rho) ## equivalent to if-else statement below
  if(runif(1) < rho){
    X[i+1] = Y
  } else{
    X[i+1] = X[i]
  }
```

```
}
```

```
mean(X)
```
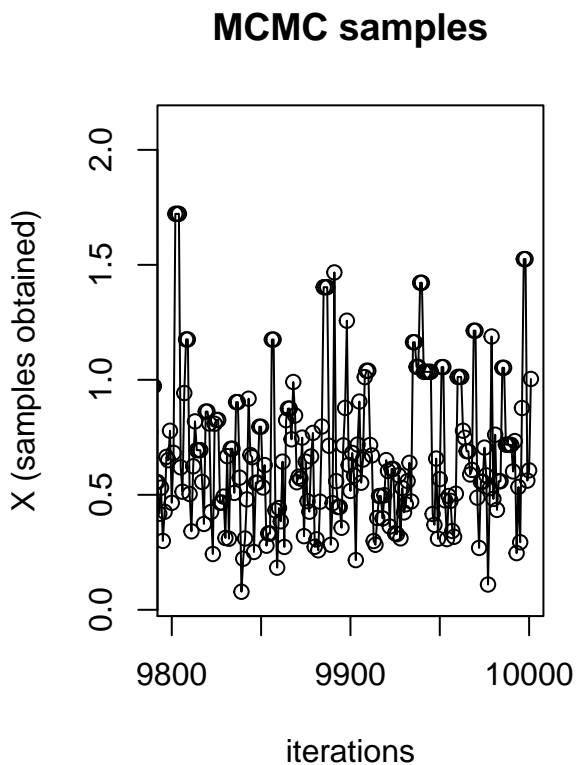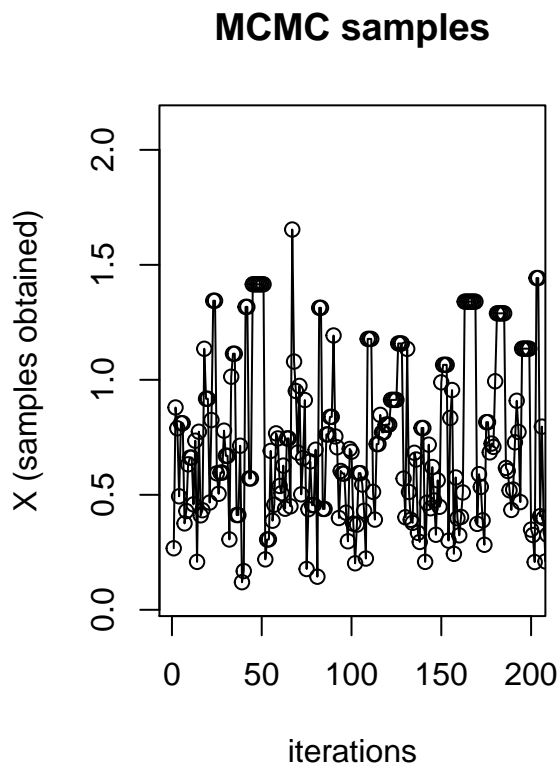
```
## [1] 0.691594
```

```
## see chain transitions
par(mfrow = c(1,2))
plot(X, type = "o", main = "MCMC samples",
     xlim = c(1,200),
     xlab = "iterations", ylab = "X (samples obtained)")

plot(X, type = "o", main = "MCMC samples",
     xlim = c(N-200,N),
     xlab = "iterations", ylab = "X (samples obtained)")
```
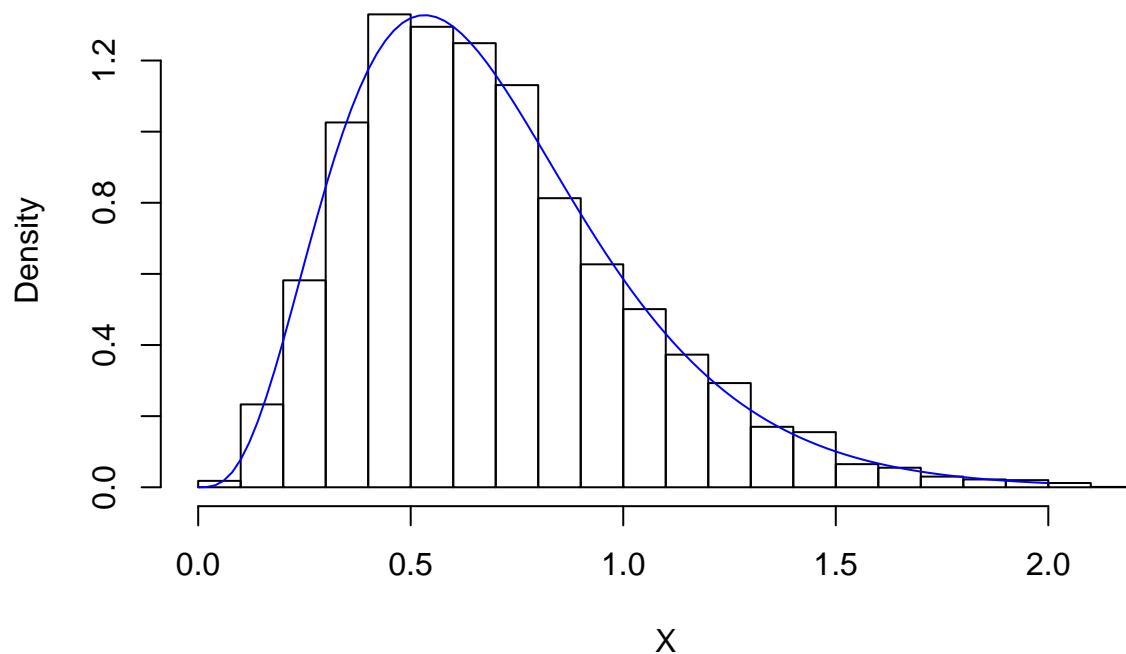


```
par(mfrow = c(1,1))
```

```
## see how samples from chain compare to Gamma density
hist(X, main = "Histogram of MCMC samples", prob = TRUE)
curve(expr = dgamma(x = x, shape = 4.3, rate = 6.2),
      from = 0, to = 2, add = TRUE, col = "blue")
```

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Histogram of MCMC samples


```r
## Metropolis Hastings
## now compare results with Gamma(5,6)

N = 10000
X = numeric(N)
X[1] = rgamma(n = 1, shape = 4.3, rate = 6.2)
for(i in 1:N){
  Y = rgamma(n = 1, shape = 5, rate = 6)
  rho = (dgamma(x = Y, shape = 4.3, rate = 6.2) * dgamma(x = X[i], shape = 5, rate = 6)) /
    (dgamma(x = X[i], shape = 4.3, rate = 6.2) * dgamma(x = Y, shape = 5, rate = 6))
  #X[i+1] = X[i] + (Y - X[i])*(runif(1) < rho) ## equivalent to if-else statement below
  if(runif(1) < rho){
    X[i+1] = Y
  } else{
    X[i+1] = X[i]
  }

}



mean(X)
```
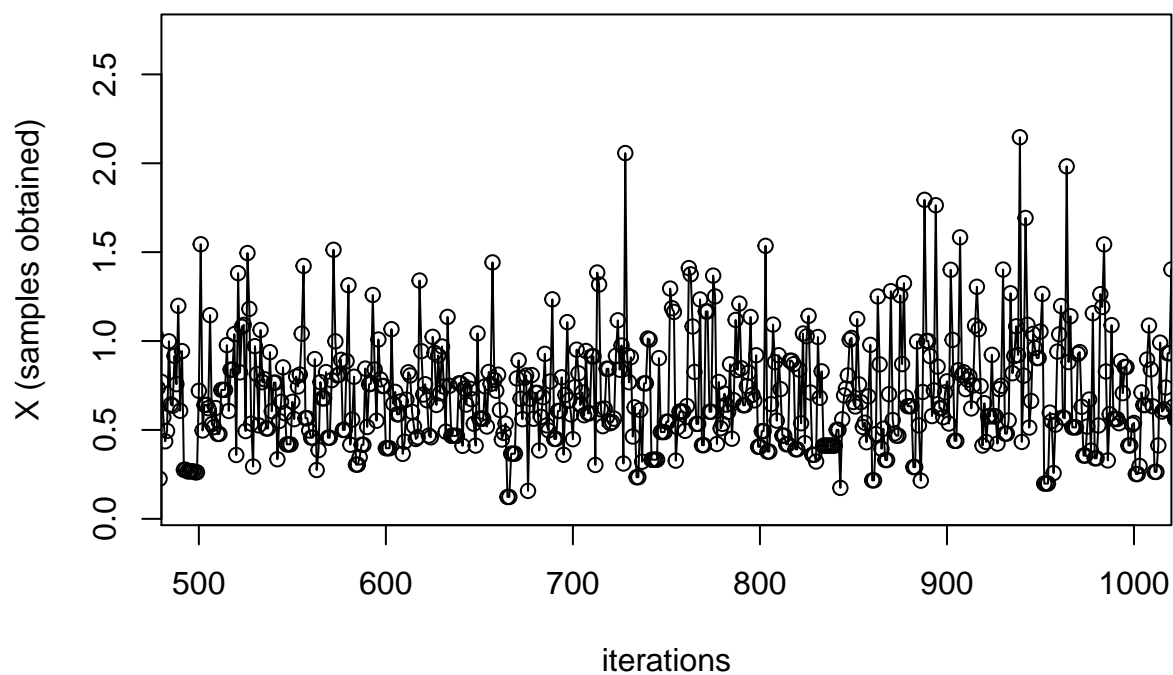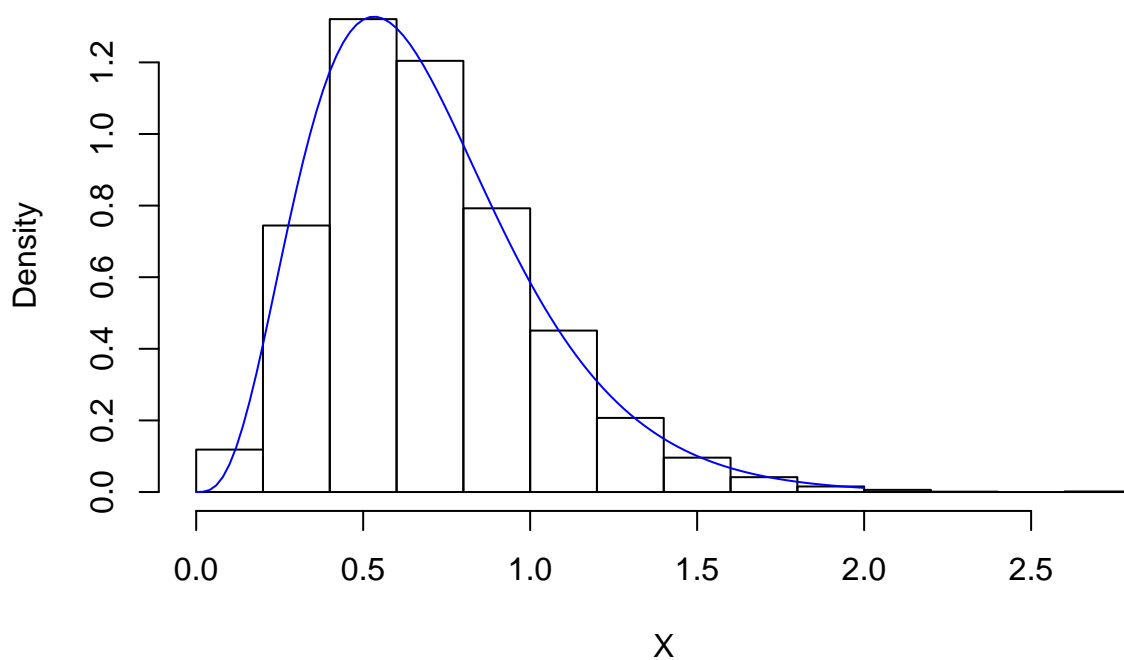
```
## [1] 0.6943115
```

```r
## see chain transitions
plot(X, type = "o", main = "MCMC samples",
     xlim = c(500,1000),
     xlab = "iterations", ylab = "X (samples obtained)")
```

MCMC samples


```
## see how samples from chain compare to Gamma density
hist(X, main = "Histogram of MCMC samples", prob = TRUE)
curve(expr = dgamma(x = x, shape = 4.3, rate = 6.2),
      from = 0, to = 2, add = TRUE, col = "blue")
```

Histogram of MCMC samples

Example 3: Rayleigh distribution

Use the M-H algorithm to generate samples from a Rayleigh distrubition. The Rayleigh density is

$$f(x) = \frac{x}{\sigma^2} e^{-x^2/(2\sigma^2)} \text{ , given that } x \geq 0, \ \sigma > 0$$

We will use the χ^2 distribution as a candidate distribution to sample from.

```r
dRayleigh = function(x, sigma = 4){
  if(any(x < 0)){
    out = 0
  } else{
  out = (x/sigma^2) * exp(-x^2 / (2 * sigma^2))
  }
  return(out)
}


N = 10000

X = numeric(N)
X[1] = 2 ## some random value

for(i in 1:N){
  Y = rchisq(n = 1, df = X[i])
  U = runif(1)
  rho = (dRayleigh(Y) * dchisq(x = X[i], df = Y)) /
        (dRayleigh(X[i]) * dchisq(x = Y, df = X[i]))
  if(U < rho){
    X[i+1] = Y
  } else {
    X[i+1] = X[i]
  }
}



## see how samples from chain compare to Gamma density
hist(X, main = "Histogram of MCMC samples", prob = TRUE)
curve(expr = dRayleigh,
      from = 0, to = 20, add = TRUE, col = "blue")
```

Histogram of MCMC samples