Simulation

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Agenda

- Simulating from distributions
- Quantile transform method
- Rejection sampling

Simulation

- Why simulate?
  - We want to see what a probability model actually does
  - We want to understand how our procedure works on a test case
  - We want to use a partly-random procedure
- All of these require drawing random variables from distributions

Simulation

- We have seen R has built in distributions: `beta`, `binom`, `cauchy`, `chisq`, `exp`, `f`, `gamma`, `geom`, `hyper`, `logis`, `lnorm`, `nbinom`, `norm`, `pois`, `t`, `tukey`, `unif`, `weibull`, `wilcox`, `signrank`
- Every distribution that R handles has four functions.
  - `p` for "probability", the cumulative distribution function (c. d. f.)
  - `q` for "quantile", the inverse c. d. f.
  - `d` for "density", the density function (p. f. or p. d. f.)
  - `r` for "random", a random variable having the specified distribution

Simulation

- Usually, R gets Uniform$(0, 1)$ random variates via a pseudorandom generator, e.g. the linear congruential generator
- Uses a sequence of Uniform$(0, 1)$ random variates to generate other distributions
- How?

Example: Binomial

- Suppose we want to generate a Binomial$(1, 1/3)$ using a $U \sim \text{Uniform}(0, 1)$
- Consider the function $X^* = I(0 < u < 1/3)$, then

  $$P(X^* = 1) = P(I(0 < u < 1/3 = 1) = P(u \in (0, 1/3)) = 1/3$$

  and $P(X^* = 0) = 2/3$
- Hence, $X^* \sim \text{Binomial}(1, 1/3)$
- Two ways to extend this to Binomial$(n, 1/3)$

Example: Binomial

```r
my.binom.1 <- function(n=1, p=1/3){
  u <- runif(n)
  binom <- sum(u<p)
  return(binom)
}

my.binom.1(1000)
```

```
## [1] 339
```

```r
my.binom.1(1000, .5)
```

```
## [1] 486
```

Example: Binomial

```
my.binom.2 <- function(n=1, p=1/3){
  u <- runif(1)
  binom <- qbinom(u, size=n, prob=p)
  return(binom)
}

my.binom.2(1000)
```

```
## [1] 361
```

```
my.binom.2(1000, .5)
```

```
## [1] 508
```

Quantile transform method

- Given $U \sim \text{Uniform}(0, 1)$ and CDF F from a continuous distribution. Then $X = F^{-1}(U)$ is a random variable with CDF F.
- Proof

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

- F^{-1} is the quantile function
- If we can generate uniforms and calculate quantiles, we can generate non-uniforms
- Also known as the Probability Integral Transform Method

Example: Exponential

- Suppose $X \sim \text{Exp}(\beta)$. Then we have density

$$f(x) = \beta^{-1} e^{-x/\beta} I(0 < x < \infty)$$

  and CDF

$$F(x) = 1 - e^{-x/\beta}$$

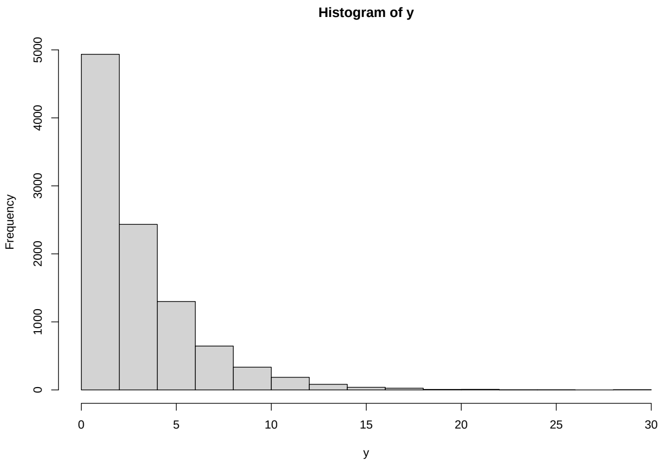
- Also

$$y = 1 - e^{-x/\beta} \text{ iff } -x/\beta = \log(1-y) \text{ iff } x = -\beta \log(1-y).$$

- Thus, $F^{-1}(y) = -\beta \log(1-y)$.
- So if $U \sim \text{Uniform}(0, 1)$, then $F^{-1}(u) = -\beta \log(1-u) \sim \text{Exp}(\beta)$.

Example: Exponential

```r
x <- runif(10000)
y <- - 3 * log(1-x)
hist(y)
```

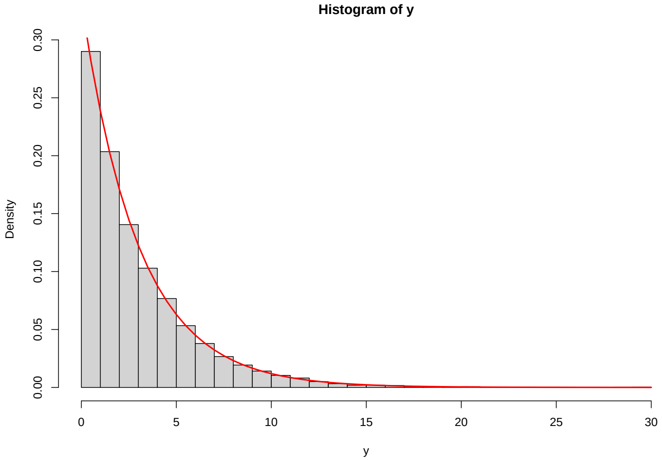



```r
mean(y)
```

```
## [1] 2.973134
```

Example: Exponential

```
true.x <- seq(0,30, .5)
true.y <- dexp(true.x, 1/3)
hist(y, freq=F, breaks=30)
points(true.x, true.y, type="l", col="red", lw=2)
```



Example: Gamma

- Remember that if $X_1, \ldots, X_n$ are IID Exp(β), then $\sum_{i=1}^{n} X_i \sim \Gamma(n, \beta)$
- Hence if we need a $\Gamma(\alpha, \beta)$ random variate and $\alpha \in \{1, 2, \ldots\}$, then take $U_1, \ldots, U_\alpha$ IID Uniform$(0, 1)$ and set

$$\sum_{i=1}^{\alpha} -\beta \log(1 - u_i) \sim \Gamma(\alpha, \beta)$$

- What if α is not an integer?

Quantile transform method

- Quantile functions often don't have closed form solutions or even nice numerical solutions
- But we know the probability density function — can we use that?

Rejection sampling

- The *accept-reject algorithm* is an indirect method of simulation
- Uses draws from a density $f_y(y)$ to get draws from $f_x(x)$
- Sampling from the wrong distribution and correcting it

Rejection sampling

Theorem: Let $X \sim f_x$ and $Y \sim f_y$ where the two densities have common support. Define

$$M = \sup_x \frac{f_x(x)}{f_y(x)}.$$

If $M < \infty$ then we can generate $X \sim f_x$ as follows,

1. Generate $Y \sim f_y$ and independently draw $U \sim \text{Uniform}(0, 1)$
2. If
$$u < \frac{f_x(y)}{M f_y(y)}$$
set $X = Y$; otherwise return to 1.

- Exercise: Why is $M \geq 1$?

Rejection sampling

- Proof

$$
\begin{aligned}
P(X \le x) &= P\left(Y \le x \mid \mathrm{STOP}\right) \\
&= P\left(Y \le x \,\middle|\, u \le \frac{f_x(y)}{Mf_y(y)}\right) \\
&= \frac{P\left(Y \le x, u \le \frac{f_x(y)}{Mf_y(y)}\right)}{P\left(u \le \frac{f_x(y)}{Mf_y(y)}\right)} \\
&= \frac{A}{B}
\end{aligned}
$$

Rejection sampling

- Now, we have

$$
\begin{aligned}
A &= P\left(Y \leq x, u \leq \frac{f_x(y)}{Mf_y(y)}\right) \\
&= E\left[P\left(Y \leq x, u \leq \frac{f_x(y)}{Mf_y(y)}\right) \,\middle|\, y\right] \\
&= E\left[I(y \leq x)\frac{f_x(y)}{Mf_y(y)}\right] \\
&= \int_{-\infty}^{\infty} I(y \leq x)\frac{f_x(y)}{Mf_y(y)} f_y(y)dy \\
&= \frac{1}{M}\int_{-\infty}^{x} f_x(y)dy = \frac{F_x(x)}{M}
\end{aligned}
$$

Rejection sampling

- Similarly, we have

$$
\begin{aligned}
B &= P\left(u \leq \frac{f_x(y)}{Mf_y(y)}\right) \\
&= E\left[P\left(u \leq \frac{f_x(y)}{Mf_y(y)}\right) \,\middle|\, y\right] \\
&= E\left[\frac{f_x(y)}{Mf_y(y)}\right] \\
&= \int_{-\infty}^{\infty} \frac{f_x(y)}{Mf_y(y)} f_y(y) dy \\
&= \frac{1}{M} \int_{-\infty}^{\infty} f_x(y) dy = \frac{1}{M}
\end{aligned}
$$

Rejection sampling

- Hence,
$$\begin{aligned} P(X \leq x) &= \frac{A}{B} \\ &= \frac{\frac{F_x(x)}{M}}{\frac{1}{M}} = F_x(x) \end{aligned}$$
- And the proof is complete. That is, $X \sim f_x$.

Rejection sampling

- Notice,

$$P(\text{STOP}) = B = P\left(u \leq \frac{f_x(y)}{Mf_y(y)}\right) = \frac{1}{M}$$

- Thus the number of iterations until the algorithm stops is Geometric$(1/M)$
- Hence, the expected number of iterations until acceptance is M.

Example: Gamma

- Suppose we want to simulate $X \sim \Gamma(3/2, 1)$ with density

$$f_x(x) = \frac{2}{\pi}\sqrt{x}e^{-x}I(0 < x < \infty).$$

- Can use the accept-reject algorithm with a $\Gamma(n, 1)$ and $n \in \{1, 2, \dots\}$ since we know how to simulate this

Example: Gamma

- Then we have

$$
\begin{aligned}
M &= \sup_{x>0} \frac{f_x(x)}{f_y(x)} \\
&= \sup_{x>0} \frac{\frac{2}{\pi}\sqrt{x}e^{-x}}{\frac{1}{(n-1)!}x^{n-1}e^{-x}} \\
&= c \sup_{x>0} x^{-n+3/2} = \infty
\end{aligned}
$$

since

$$n < 3/2 \text{ implies } x^{-n+3/2} \to \infty \text{ as } x \to \infty$$

and

$$n > 3/2 \text{ implies } x^{-n+3/2} \to \infty \text{ as } x \to 0$$

Example: Gamma

- Hence, we need to be a little more creative with our proposal distribution
- We could consider a mixture distribution. That is, if $f_1(z)$ and $f_2(z)$ are both densities and $p \in [0, 1]$. Then

$$pf_1(z) + (1-p)f_2(z)$$

  is also a density
- Consider a proposal that is a mixture of a $\Gamma(1, 1) = \text{Exp}(1)$ and a $\Gamma(2, 1)$, i.e.

$$f_y(y) = \left[pe^{-y} + (1-p)ye^{-y}\right] I(0 < y < \infty)$$

Example: Gamma

- Now, we have

$$\begin{aligned} M &= \sup_{x>0} \frac{f_x(x)}{f_y(x)} \\ &= \sup_{x>0} \frac{\frac{2}{\sqrt{\pi}}\sqrt{x}e^{-x}}{pe^{-x} + (1-p)xe^{-x}} \\ &= \frac{2}{\sqrt{\pi}} \sup_{x>0} \frac{\sqrt{x}}{p + (1-p)x} \\ &= \frac{2}{\sqrt{\pi}} \frac{1}{2\sqrt{p(1-p)}} \end{aligned}$$

- Exercise: Prove the last line, i.e. maximize $h(x) = \frac{\sqrt{x}}{p+(1-p)x}$ for $x > 0$ or $\log h(x)$.

Example: Gamma

- Note that M is minimized when $p = 1/2$ so that $M_{1/2} = 2/\sqrt{\pi} \approx 1.1283$.
- Then the accept-reject algorithm to simulate $X \sim \Gamma(3/2, 1)$ is as follows

1. Draw $Y \sim f_y$ with

$$f_y(y) = \left[pe^{-y} + (1-p)ye^{-y}\right] I(0 < y < \infty)$$

   and and independently draw $U \sim \text{Uniform}(0, 1)$
2. If

$$u < \frac{2}{\sqrt{\pi}} \frac{f_x(y)}{f_y(y)} = \frac{2\sqrt{y}}{1+y}$$

   set $X = Y$; otherwise return to 1

Simulating from mixtures

- Write $f(z) = pf_1(z) + (1-p)f_2(z)$ as the marginal of the joint given by

$$f(z|w) = f_1(z)I(w=1) + f_2(z)I(w=0)$$

  where $W \sim \text{Binomial}(1, p)$
- Thus to simulate from $f(z)$

1. Draw $U \sim \text{Uniform}(0, 1)$
2. If $u < p$ take $Z \sim f_1(z)$; otherwise take $Z \sim f_2(z)$

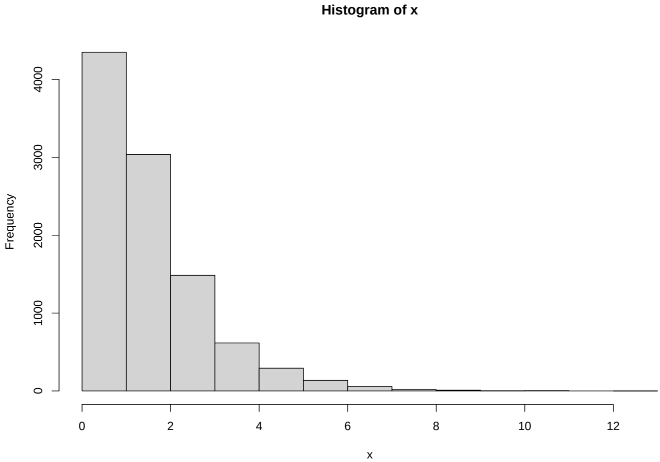
- Exercise: Show $Z \sim f(z)$

Example: Gamma

```
ar.gamma <- function(n=100){
x <- double(n)
i <- 1
while(i < (n+1)) {
    u <- runif(1)
    if(u < .5){
        y <- -1 * log(1-runif(1))
    } else {
        y <- sum(-1 * log(1-runif(2)))
    }
    u <- runif(1)
    temp <- 2 * sqrt(y) / (1+y)
    if(u < temp){
        x[i] <- y
        i <- i+1
    }
}
return(x)
}
```

Example: Gamma

```r
x <- ar.gamma(10000)
hist(x)
```

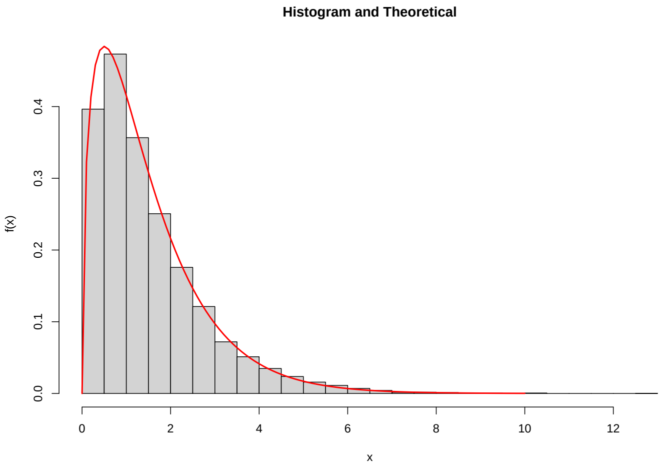



```r
mean(x)
```

```
## [1] 1.509658
```

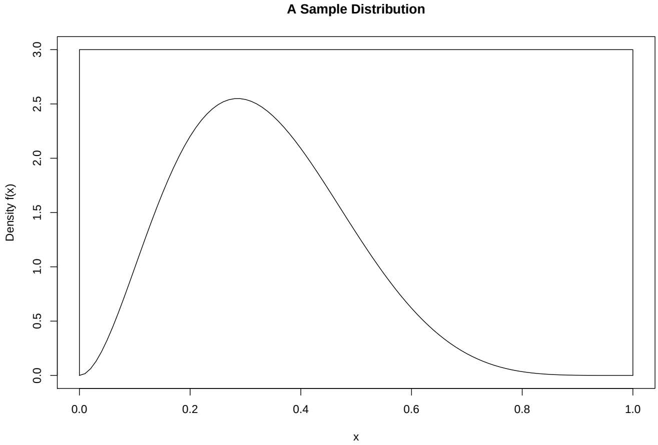
Example: Gamma

```r
true.x <- seq(0,10, .1)
true.y <- dgamma(true.x, 3/2, 1)
hist(x, freq=F, breaks=30, xlab="x", ylab="f(x)", main="Histogram and Theoretical")
points(true.x, true.y, type="l", col="red", lw=2)
```



Example: Beta

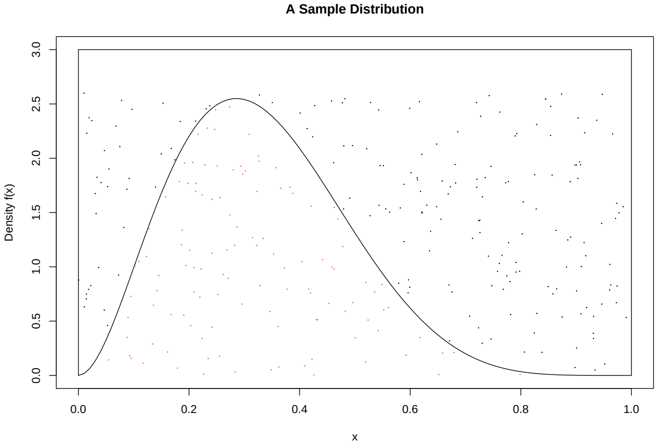
- Suppose the pdf f is zero outside an interval $[c, d]$, and $\leq M$ on the interval.



Example: Beta

- We know how to draw from uniform distributions in any dimension. Do it in two:

```r
x1 <- runif(300, 0, 1); y1 <- runif(300, 0, 2.6);
selected <- y1 < dbeta(x1, 3, 6)
```



Example: Beta

```r
mean(selected)
```

```
## [1] 0.3866667
```

```r
accepted.points <- x1[selected]
mean(accepted.points < 0.5)
```

```
## [1] 0.8706897
```

```r
pbeta(0.5, 3, 6)
```

```
## [1] 0.8554688
```

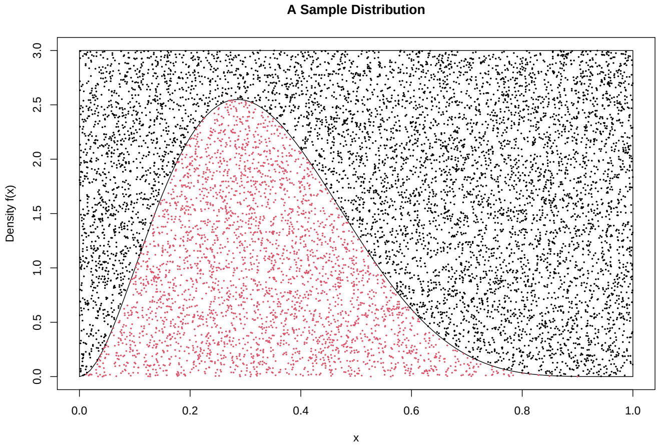
Example: Beta

- For this to work efficiently, we have to cover the target distribution with one that sits close to it.

```
x2 <- runif(10000, 0, 1); y2 <- runif(10000, 0, 3);
selected <- y2 < dbeta(x2, 3, 6)
mean(selected)
```

```
## [1] 0.3245
```

Example: Beta



Alternatives

- Squeezed rejection sampling may help if evaluating f is expensive
- Adaptive rejection sampling may help generate an envelope
- ...

Box-Muller

- **Box-Muller transformation** transform generates pairs of independent, standard normally distributed random numbers, given a source of uniformly distributed random numbers
- Let $U \sim \text{Uniform}(0, 1)$ and $V \sim \text{Uniform}(0, 1)$ and set

$$R = \sqrt{-2 \log U} \qquad \text{and} \qquad \theta = 2\pi V$$

- Then the following transformation yields two independent normal random variates

$$X = R \cos(\theta) \qquad \text{and} \qquad Y = R \sin(\theta)$$

Summary

- Can transform uniform draws into other distributions when we can compute the distribution function
  - Quantile method when we can invert the CDF
  - The rejection method if all we have is the density
- Basic R commands encapsulate a lot of this for us
- Optimized algorithms based on distribution and parameter values

Exercise: Box-Muller

1. Write a function named `bmnormal` that simulates `n` draws from Normal random variable with mean `mu` and standard deviation `sd` using the Box-Muller transformation.
2. Inputs to your function should be `n`, `mu`, and `sd`.
3. Simulate 2000 draws from a Normal with mean 10 and standard deviation 3.
4. Convince yourself with a plot your sampler is working correctly. Is there a test you could consider also?