Chapter 13 Introduction to Simulation Using R

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13.1 Analysis versus Computer Simulation

A computer simulation is a computer program which attempts to represent the real world based on a model. The accuracy of the simulation depends on the precision of the model. Suppose that the probability of heads in a coin toss experiment is unknown. We can perform the experiment of tossing the coin n times repetitively to approximate the probability of heads.

 $P(H) = \frac{\text{Number of times heads observed}}{\text{Number of times the experiment executed}}$

However, for many practical problems it is not possible to determine the probabilities by executing experiments a large number of times. With today's computers processing capabilities, we only need a high-level language, such as R, which can generate random numbers, to deal with these problems.

In this chapter, we present basic methods of generating random variables and simulate probabilistic systems. The provided algorithms are general and can be implemented in any computer language. However, to have concrete examples, we provide the actual codes in R. If you are unfamiliar with R, you should still be able to understand the algorithms.

13.2 Introduction: What is R?

R is a programming language that helps engineers and scientists find solutions for given statistical problems with fewer lines of codes than traditional programming languages, such as C/C++ or Java, by utilizing built-in statistical functions. There are many built-in statistical functions and add-on packages available in R. It also has high quality customizable graphics capabilities. R is available for Unix/Linux, Windows, and Mac. Besides all these features, R is free!

13.3 Discrete and Continuous Random Number Generators

Most of the programming languages can deliver samples from the uniform distribution to us (In reality, the given values are pseudo-random instead of being completely random.) The rest of this section shows how to convert uniform random variables to any other desired random variable. The R code for generating uniform random variables is:

U = runif(n, min = 0, max = 1)

which returns a pseudorandom value drawn from the standard uniform distribution on the open interval (0,1).

13.3.1 Generating Discrete Probability Distributions from Uniform Distribution

Let's see a few examples of generating certain simple distributions:

Example 1. (Bernoulli) Simulate tossing a coin with probability of heads *p*.

Solution: Let U be a Uniform(0,1) random variable. We can write Bernoulli random variable X as:

$$X = \begin{cases} 1 & U$$

Thus,

$$P(H) = P(X = 1)$$
$$= P(U < p)$$
$$= p$$

Therefore, X has Bernoulli(p) distribution. The R code for Bernoulli(0.5) is:

p = 0.5; U = runif(1, min = 0, max = 1);X = (U < p);

Since the "runif(1, min = 0, max = 1)" command returns a number between 0 and 1, we divided the interval [0, 1] into two parts, p and 1-p in length. Then, the value of X is determined based on where the number generated from uniform distribution fell.

Example 2. (Coin Toss Simulation) Write codes to simulate tossing a fair coin to see how the law of large numbers works.

Solution: You can write:

```
\begin{split} n &= 1000; \\ U &= runif(n, min = 0, max = 1); \\ toss &= U < 0.5; \\ a &= numeric(n + 1); \\ avg &= numeric(n); \\ for(i \ in \ 2:n + 1) \\ \{ \\ a[i] &= a[i - 1] + toss[i - 1]; \\ avg[i - 1] &= a[i]/(i - 1); \\ \} \\ plot(1:n, avg[1:n], type = "l", lwd = 5, col = "blue", ylab = "Proportion of Heads", \\ xlab = "CoinTossNumber", cex.main = 1.25, cex.lab = 1.5, cex.axis = 1.75) \end{split}
```

If you run the above codes to compute the proportion of ones in the variable "toss," the result will look like Figure 13.1. You can also assume the coin is unbiased with probability of heads equal to 0.6 by replacing the third line of the previous code with:



Figure 13.1: R - coin toss simultion

Example 3. (Binomial) Generate a Binomial(50, 0.2) random variable.

Solution: To solve this problem, we can use the following lemma:

Lemma 1. If $X_1, X_2, ..., X_n$ are independent Bernoulli(p) random variables, then the random variable X defined by $X = X_1 + X_2 + ... + X_n$ has a Binomial(n, p) distribution.

To generate a random variable $X \sim Binomial(n, p)$, we can toss a coin n times and count the number of heads. Counting the number of heads is exactly the same as finding $X_1 + X_2 + ... + X_n$, where each X_i is equal to one if the corresponding coin toss results in heads and zero otherwise.

Since we know how to generate Bernoulli random variables, we can generate a Binomial(n, p) by adding n independent Bernoulli(p) random variables.

p = 0.2; n = 50; U = runif(n, min = 0, max = 1);X = sum(U < p);

Generating Arbitrary Discrete Distributions

In general, we can generate any discrete random variables similar to the above examples using the following algorithm. Suppose we would like to simulate the discrete random variable X with range $R_X = \{x_1, x_2, ..., x_n\}$ and $P(X = x_j) = p_j$, so $\sum_j p_j = 1$.

To achieve this, first we generate a random number U (i.e., $U \sim Uniform(0,1)$). Next, we divide the interval [0,1] into subintervals such that the *j*th subinterval has length p_j (Figure 13.2). Assume

$$X = \begin{cases} x_0 & \text{if } (U < p_0) \\ x_1 & \text{if } (p_0 \le U < p_0 + p_1) \\ \vdots \\ x_j & \text{if } (\sum_{k=0}^{j-1} p_k \le U < \sum_{k=0}^j p_k \\ \vdots \end{cases}$$

In other words

$$X = x_j \quad \text{if} \quad F(x_{j-1}) \le U < F(x_j),$$

where F(x) is the desired CDF. We have

$$P(X = x_j) = P\left(\sum_{k=0}^{j-1} p_k \le U < \sum_{k=0}^{j} p_k\right)$$
$$= p_j$$



Example 4. Give an algorithm to simulate the value of a random variable X such that

P(X = 1) = 0.35P(X = 2) = 0.15P(X = 3) = 0.4P(X = 4) = 0.1

Solution: We divide the interval [0, 1] into subintervals as follows:

$$A_0 = [0, 0.35)$$
$$A_1 = [0.35, 0.5)$$
$$A_2 = [0.5, 0.9)$$
$$A_3 = [0.9, 1)$$

Subinterval A_i has length p_i . We obtain a uniform number U. If U belongs to A_i , then $X = x_i$.

$$P(X = x_i) = P(U \in A_i)$$
$$= p_i$$

P = c(0.35, 0.5, 0.9, 1); X = c(1, 2, 3, 4); counter = 1; r = runif(1, min = 0, max = 1); while(r > P[counter]) counter = counter + 1; endX[counter]

13.3.2 Generating Continuous Probability Distributions from the Uniform Distribution- Inverse Transformation Method

At least in principle, there is a way to convert a uniform distribution to any other distribution. Let's see how we can do this. Let $U \sim Uniform(0,1)$ and F be a CDF. Also, assume F is continuous and strictly increasing as a function. **Theorem 1.** Let $U \sim Uniform(0,1)$ and F be a CDF which is strictly increasing. Also, consider a random variable X defined as

$$X = F^{-1}(U).$$

Then,

$$X \sim F$$
 (The CDF of X is F)

Proof:

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

= $P(U \le F(x))$ (increasing function)
= $F(x)$

Now, let's see some examples. Note that to generate any continuous random variable X with the continuous cdf F, $F^{-1}(U)$ has to be computed.

Example 5. (Exponential) Generate an Exponential(1) random variable.

Solution: To generate an Exponential random variable with parameter $\lambda = 1$, we proceed as follows

$$F(x) = 1 - e^{-x} \qquad x > 0$$
$$U \sim Uniform(0, 1)$$
$$X = F^{-1}(U)$$
$$= -\ln(1 - U)$$
$$X \sim F$$

This formula can be simplified since

$$1 - U \sim Uniform(0, 1)$$
$$\underbrace{ \begin{array}{c} U \\ U \\ 0 \end{array}}_{1} 1 - U \xrightarrow{1}_{1} 0$$

Figure 13.3: Symmetry of Uniform

Hence we can simulate X using

$$X = -\ln(U)$$

$$U = runif(1, min = 0, max = 1);$$

$$X = -log(U)$$

Example 6. (Gamma) Generate a Gamma(20,1) random variable.

Solution: For this example, F^{-1} is even more complicated than the complicated gamma cdf F itself. Instead of inverting the CDF, we generate a gamma random variable as a sum of n independent exponential variables.

Theorem 2. Let X_1, X_2, \dots, X_n be independent random variables with $X_i \sim Exponential(\lambda)$. Define

$$Y = X_1 + X_2 + \dots + X_n$$

By the moment generating function method, you can show that Y has a gamma distribution with parameters n and λ , i.e., $Y \sim Gamma(n, \lambda)$.

Having this theorem in mind, we can write:

$$\begin{split} n &= 20;\\ lambda &= 1;\\ X &= (-1/lambda) * sum(log(runif(n, min = 0, max = 1))); \end{split}$$

Example 7. (Poisson) Generate a Poisson random variable. Hint: In this example, use the fact that the number of events in the interval [0, t] has Poisson distribution when the elapsed times between the events are Exponential.

Solution: We want to employ the definition of Poisson processes. Assume N represents the number of events (arrivals) in [0,t]. If the interarrival times are distributed exponentially (with parameter λ) and independently, then the number of arrivals occurred in [0,t], N, has Poisson distribution with parameter λt (Figure 13.4). Therefore, to solve this problem, we can repeat generating $Exponential(\lambda)$ random variables while their sum is not larger than 1 (choosing t = 1). More specifically, we generate $Exponential(\lambda)$ random variables

$$T_i = \frac{-1}{\lambda} \ln(U_i)$$

by first generating uniform random variables U_i 's. Then we define

$$X = \max\left\{j: T_1 + \dots + T_j \le 1\right\}$$

The algorithm can be simplified:

$$X = \max\left\{j : \frac{-1}{\lambda}\ln(U_1\cdots U_j) \le 1\right\}$$

```
\begin{split} Lambda &= 2; \\ i &= 0; \\ U &= runif(1, min = 0, max = 1); \\ Y &= -(1/Lambda) * log(U); \\ sum &= Y; \\ while(sum < 1) \\ \{U &= runif(1, min = 0, max = 1); \\ Y &= -(1/Lambda) * log(U); \\ sum &= sum + Y; \\ i &= i + 1; \} \\ X &= i \end{split}
```





To finish this section, let's see how to convert uniform numbers to normal random variables. Normal distribution is extremely important in science because it is very commonly occuring.

Theorem 3. (Box-Muller transformation) We can generate a pair of independent normal variables (Z_1, Z_2) by transforming a pair of independent Uniform(0, 1) random variables (U_1, U_2) [1].

$$\begin{cases} Z_1 = \sqrt{-2\ln U_1} \cos(2\pi U_2) \\ Z_2 = \sqrt{-2\ln U_1} \sin(2\pi U_2) \end{cases}$$

Example 8. (Box-Muller) Generate 5000 pairs of normal random variables and plot both histograms.

Solution: We display the pairs in Matrix form.

13.4. R COMMANDS FOR SPECIAL DISTRIBUTIONS





Figure 13.5: Histogram of Z1, a normal random variable generated by Box-Muller transformation

13.4 R Commands for Special Distributions

In this section, we will see some useful commands for commonly employed distributions. Functions which start with "p", "q", "d", and "r" give the cumulative distribution function (CDF), the inverse CDF, the density function (PDF), and a random variable having the specified distribution respectively.

Distributions

Commands

Binomial	pbinom	qbinom	dbinom	rbinom
Geometric	pgeom	qgeom	dgeom	rgeom
Negative Binomial	pnbinom	qnbinom	dnbinom	rnbinom
Poisson	ppois	qpois	dpois	rpois
Beta	pbeta	qbeta	dbeta	rbeta
Beta	pbeta	qbeta	dbeta	rbeta
Exponential	pexp	qexp	dexp	rexp
Gamma	pgamma	qgamma	dgamma	rgamma
Studentt	pt	qt	dt	rt
Uniform	punif	qunif	dunif	runif

13.5 Exercises

1. Write R programs to generate Geometric(p) and Negative Binomial(i,p) random variables.

Solution: To generate a Geometric random variable, we run a loop of Bernoulli trials until the first success occurs. K counts the number of failures plus one success, which is equal to the total number of trials.

$$\begin{split} K &= 1;\\ p &= 0.2;\\ while(runif(1) > p)\\ K &= K + 1;\\ K \end{split}$$

Now, we can generate Geometric random variable i times to obtain a Negative Binomial(i, p) variable as a sum of i independent Geometric (p) random variables.

$$\begin{split} &K = 1; \\ &p = 0.2; \\ &r = 2; \\ &success = 0; \\ &while(success < r) \\ &\{if \quad (runif(1) > p) \\ &\{K = K + 1; \\ &print = 0 \quad \#Failure \\ &\}else \\ &\{success = success + 1; \\ &print = 1\}\} \quad \#Success \\ &K + r - 1 \quad \#Number \quad of \quad trials \quad needed \quad to \quad obtain \quad r \quad successes \end{split}$$

2. (Poisson) Use the algorithm for generating discrete random variables to obtain a Poisson random variable with parameter $\lambda = 2$.

Solution: We know a Poisson random variable takes all nonnegative integer values with probabilities

$$p_i = P(X = x_i) = e^{-\lambda} \frac{\lambda^i}{i!}$$
 for $i = 0, 1, 2, \cdots$

To generate a $Poisson(\lambda)$, first we generate a random number U. Next, we divide the interval [0, 1] into subintervals such that the *j*th subinterval has length p_j (Figure 13.2). Assume

$$X = \begin{cases} x_0 & \text{if } (U < p_0) \\ x_1 & \text{if } (p_0 \le U < p_0 + p_1) \\ \vdots \\ x_j & \text{if } (\sum_{k=0}^{j-1} p_k \le U < \sum_{k=0}^j p_k) \\ \vdots \end{cases}$$

Here $x_i = i - 1$, so

$$X = i \quad \text{if} \quad p_0 + \dots + p_{i-1} \le U < p_0 + \dots + p_{i-1} + p_i$$
$$F(i-1) \le U < F(i) \quad \text{F is CDF}$$

$$\begin{split} lambda &= 2; \\ i &= 0; \\ U &= runif(1); \\ cdf &= exp(-lambda); \\ while(U >= cdf) \\ \{i &= i+1; \\ cdf &= cdf + exp(-lambda) * lambda^{i}/gamma(i+1); \} \\ X &= i; \end{split}$$

3. Explain how to generate a random variable with the density

$$f(x) = 2.5x\sqrt{x} \quad \text{for} \quad 0 < x < 1$$

if your random number generator produces a Standard Uniform random variable U. Hint: use the inverse transformation method.

Solution:

$$F_X(X) = X^{\frac{5}{2}} = U \quad (0 < x < 1)$$

 $X = U^{\frac{2}{5}}$

$$\begin{split} U &= runif(1);\\ X &= U^{\frac{2}{5}}; \end{split}$$

We have the desired distribution.

4. Use the inverse transformation method to generate a random variable having distribution function

$$F(x) = \frac{x^2 + x}{2}, \quad 0 \le x \le 1$$

Solution:

$$\frac{X^2 + X}{2} = U$$

$$(X + \frac{1}{2})^2 - \frac{1}{4} = 2U$$

$$X + \frac{1}{2} = \sqrt{2U + \frac{1}{4}}$$

$$X = \sqrt{2U + \frac{1}{4}} - \frac{1}{2} \quad (X, U \in [0, 1])$$

13.5. EXERCISES

By generating a random number, U, we have the desired distribution.

$$U = runif(1);$$

$$X = sqrt\left(2U + \frac{1}{4}\right) - \frac{1}{2};$$

5. Let X have a standard Cauchy distribution.

$$F_X(x) = \frac{1}{\pi}\arctan(x) + \frac{1}{2}$$

Assuming you have $U \sim Uniform(0, 1)$, explain how to generate X. Then, use this result to produce 1000 samples of X and compute the sample mean. Repeat the experiment 100 times. What do you observe and why?

Solution: Using Inverse Transformation Method:

$$U - \frac{1}{2} = \frac{1}{\pi} \arctan(X)$$
$$\pi \left(U - \frac{1}{2}\right) = \arctan(X)$$
$$X = \tan\left(\pi(U - \frac{1}{2})\right)$$

Next, here is the R code:

```
\begin{split} &U = numeric(1000); \\ &n = 100; \\ &average = numeric(n); \\ &for \quad (i \quad in \quad 1:n) \\ &\{U = runif(1000); \\ &X = tan(pi * (U - 0.5)); \\ &average[i] = mean(X); \\ &plot(1:n, average[1:n], type = "l", lwd = 2, col = "blue") \end{split}
```

Cauchy distribution has no mean (Figure 13.6), or higher moments defined.

6. (The Rejection Method) When we use the Inverse Transformation Method, we need a simple form of the cdf F(x) that allows direct computation of $X = F^{-1}(U)$. When F(x) doesn't have a simple form but the pdf f(x) is available, random variables with density f(x) can be generated by the **rejection method**. Suppose you have a method



Figure 13.6: Cauchy Mean

for generating a random variable having density function g(x). Now, assume you want to generate a random variable having density function f(x). Let c be a constant such that

$$\frac{f(y)}{g(y)} \le c \quad \text{(for all y)}$$

Show that the following method generates a random variable with density function f(x).

- Generate Y having density g.
- Generate a random number U from Uniform (0, 1).
- If $U \leq \frac{f(Y)}{cg(Y)}$, set X = Y. Otherwise, return to step 1.

Solution: The number of times N that the first two steps of the algorithm need to be called is itself a random variable and has a geometric distribution with "success" probability

$$p = P\left(U \le \frac{f(Y)}{cg(Y)}\right)$$

Thus, $E(N) = \frac{1}{p}$. Also, we can compute p:

$$P\left(U \le \frac{f(Y)}{cg(Y)} | Y = y\right) = \frac{f(y)}{cg(y)}$$

$$p = \int_{-\infty}^{\infty} \frac{f(y)}{cg(y)} g(y) dy$$

$$= \frac{1}{c} \int_{-\infty}^{\infty} f(y) dy$$

$$= \frac{1}{c}$$
Therefore, $F(N)$

Therefore, E(N) = c

Let *F* be the desired CDF (CDF of *X*). Now, we must show that the conditional distribution of *Y* given that $U \leq \frac{f(Y)}{cg(Y)}$ is indeed *F*, i.e. $P(Y \leq y | U \leq \frac{f(Y)}{cg(Y)}) = F(y)$. Assume $M = \{U \leq \frac{f(Y)}{cg(Y)}\}, K = \{Y \leq y\}$. We know $P(M) = p = \frac{1}{c}$. Also, we can compute

$$\begin{split} P(U \leq \frac{f(Y)}{cg(Y)} | Y \leq y) &= \frac{P(U \leq \frac{f(Y)}{cg(Y)}, Y \leq y)}{G(y)} \\ &= \int_{-\infty}^{y} \frac{P(U \leq \frac{f(y)}{cg(y)} | Y = v \leq y)}{G(y)} g(v) dv \\ &= \frac{1}{G(y)} \int_{-\infty}^{y} \frac{f(v)}{cg(v)} g(v) dv \\ &= \frac{1}{cG(y)} \int_{-\infty}^{y} f(v) dv \\ &= \frac{F(y)}{cG(y)} \end{split}$$

Thus,

$$P(K|M) = P(M|K)P(K)/P(M)$$

= $P(U \le \frac{f(Y)}{cg(Y)}|Y \le y) \times \frac{G(y)}{\frac{1}{c}}$
= $\frac{F(y)}{cG(y)} \times \frac{G(y)}{\frac{1}{c}}$
= $F(y)$

7. Use the rejection method to generate a random variable having density function Beta(2, 4). Hint: Assume g(x) = 1 for 0 < x < 1. Solution:

> $f(x) = 20x(1-x)^3 \quad 0 < x < 1$ $g(x) = 1 \quad 0 < x < 1$ $\frac{f(x)}{g(x)} = 20x(1-x)^3$

We need to find the smallest constant c such that $f(x)/g(x) \leq c$. Differentiation of this quantity yields

$$\frac{d\left(\frac{f(x)}{g(x)}\right)}{dx} = 0$$

Thus, $x = \frac{1}{4}$
Therefore, $\frac{f(x)}{g(x)} \le \frac{135}{64}$
Hence, $\frac{f(x)}{cg(x)} = \frac{256}{27}x(1-x)^3$

- $$\begin{split} n &= 1; \\ while \quad (n == 1) \\ \{U1 = runif(1); \\ U2 = runif(1); \\ if \quad (U2 <= 256/27 * U1 * (1 U1)^{\wedge}3) \\ \{X = U1; \\ n = 0; \}\} \end{split}$$
- 8. Use the rejection method to generate a random variable having the $Gamma(\frac{5}{2}, 1)$ density function. Hint: Assume g(x) is the pdf of the $Gamma\left(\alpha = \frac{5}{2}, \lambda = 1\right)$. Solution:

$$f(x) = \frac{4}{3\sqrt{\pi}} x^{\frac{3}{2}} e^{-x}, x > 0$$

$$g(x) = \frac{2}{5} e^{-\frac{2x}{5}} \quad x > 0$$

$$\frac{f(x)}{g(x)} = \frac{10}{3\sqrt{\pi}} x^{\frac{3}{2}} e^{-\frac{3x}{5}}$$

$$\frac{d\left(\frac{f(x)}{g(x)}\right)}{dx} = 0$$
Hence, $x = \frac{5}{2}$

$$c = \frac{10}{3\sqrt{\pi}} \left(\frac{5}{2}\right)^{\frac{3}{2}} e^{\frac{-3}{2}}$$

$$\frac{f(x)}{cg(x)} = \frac{x^{\frac{3}{2}} e^{\frac{-3x}{5}}}{\left(\frac{5}{2}\right)^{\frac{3}{2}} e^{\frac{-3}{2}}}$$

We know how to generate an Exponential random variable.

13.5. EXERCISES

- Generate a random number U_1 and set $Y = -\frac{5}{2} \log U_1$.
- Generate a random number U_2 .
- If $U_2 < \frac{Y^{\frac{3}{2}}e^{\frac{-3Y}{5}}}{(\frac{5}{2})^{\frac{3}{2}}e^{\frac{-3}{2}}}$, set X = Y. Otherwise, execute the step 1.
- 9. Use the rejection method to generate a standard normal random variable. Hint: Assume g(x) is the pdf of the exponential distribution with $\lambda = 1$.

Solution:

$$f(x) = \frac{2}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \quad 0 < x < \infty$$

$$g(x) = e^{-x} \quad 0 < x < \infty \quad \text{(Exponential density function with mean 1)}$$
Thus,
$$\frac{f(x)}{g(x)} = \sqrt{\frac{2}{\pi}} e^{x - \frac{x^2}{2}}$$
Thus,
$$x = 1 \quad \text{maximizes} \quad \frac{f(x)}{g(x)}$$
Thus,
$$c = \sqrt{\frac{2e}{\pi}}$$

$$\frac{f(x)}{cg(x)} = e^{-\frac{(x-1)^2}{2}}$$

- Generate Y, an exponential random variable with mean 1.
- Generate a random number U.
- If $U \le e^{\frac{-(Y-1)^2}{2}}$ set X = Y. Otherwise, return to step 1.
- 10. Use the rejection method to generate a Gamma(2, 1) random variable conditional on its value being greater than 5, that is

$$f(x) = \frac{xe^{-x}}{\int_5^\infty xe^{-x}dx}$$
$$= \frac{xe^{-x}}{6e^{-5}} \quad (x \ge 5)$$

Hint: Assume q(x) be the density function of exponential distribution.

Solution: Since Gamma(2,1) random variable has expected value 2, we use an exponential distribution with mean 2 that is conditioned to be greater than 5.

$$f(x) = \frac{xe^{(-x)}}{\int_5^\infty xe^{(-x)}dx}$$
$$= \frac{xe^{(-x)}}{6e^{(-5)}} \quad x \ge 5$$
$$g(x) = \frac{\frac{1}{2}e^{(-\frac{x}{2})}}{e^{\frac{-5}{2}}} \quad x \ge 5$$
$$\frac{f(x)}{g(x)} = \frac{x}{3}e^{-(\frac{x-5}{2})}$$

We obtain the maximum in x = 5 since $\frac{f(x)}{g(x)}$ is decreasing. Therefore,

$$c = \frac{f(5)}{g(5)} = \frac{5}{3}$$

- Generate a random number V.
- $Y = 5 2\log(V)$.
- Generate a random number U.
- If $U < \frac{Y}{5}e^{-(\frac{Y-5}{2})}$, set X = Y; otherwise return to step 1.

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