Introduction
General techniques for simulating continuous RVs
Special techniques for simulating continuous RVs
Simulating from discrete distributions
Multivariate distributions & Stochastic Processes
Variance reduction techniques
Determining optimal number of runs

Simulation: Random Variables & Stochastic processes

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July 2013



- Introduction
 - What is Monte Carlo simulation?
- Quantum General techniques for simulating continuous RVs
 - Inverse transformation method
 - The rejection method
 - Hazard rate method
- 3 Special techniques for simulating continuous RVs
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What is Monte Carlo simulation?

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Simulating an RV

- Let $X = (X_1, X_2, \dots, X_n)$ denote a random vector
 - having density function $f(x_1, x_2, ..., x_n)$

•
$$E[g(X)] = \iint ... \int g(x_1, x_2, ..., x_n) f(x_1, x_2, ..., x_n) dx_1 dx_2, ..., dx_n$$



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- Analytical OR numerical integration is tedious
- Alternately, approximate E[g(X)] by means of SIMULATION



Approximating E[g(X)]

Monte Carlo Simulation

- Generate a random RV,
 - $\mathbf{X}^{(1)} = \left(\mathbf{X}_{1}^{(1)}, \mathbf{X}_{2}^{(1)}, \cdots, \mathbf{X}_{n}^{(1)}\right)$ having density function $f(x_{1}, x_{2}, \dots, x_{n})$
 - compute $Y^{(1)} = g(X^{(1)})$

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 - compute $Y^{(2)} = g(X^{(2)})$
- Repeat this r number of times, generating i.i.d RVs
 - $Y^{(i)} = g(X^{(i)}), i = 1, 2, ..., r$ are generated
 - $\bullet \Rightarrow \lim_{r \to \infty} \frac{Y^{(1)} + Y^{(2)} + \dots + Y^{(r)}}{r} = E[Y^{(i)}] = E[g(\mathbf{X})]$

How to generate a Random Vectors, $\mathbf{X}^{(r)}$

Generating random vectors X having specified joint distribution?

- Objective-
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Generating random vectors X having specified joint distribution?

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 - Generate a sequence of random vectors $\mathbf{X}^{(r)}$ having aprticular distribution.
- As first step, we need to be able to generate random variables from uniform distribution (0,1)

Generating a Uniform RV on (0,1), MANUALLY

- 10 identical slips, containing numbers 0..9

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Generating a Uniform RV on (0,1), MANUALLY

- 10 identical slips, containing numbers 0..9
- Successively select, n chits with replacement
- Equivalent to generating a string of *n* digits with decimal in front, thus can be regarded as a value of a uniform (0,1) RV rounded off to nearest $\left(\frac{1}{10}\right)^n$

What is Monte Carlo simulation?

Generating random variable on UNIFORM (0,1)

- Pseudo random instead of truly random



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- Then, recursively compute values using a, c and m
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Inverse transform method

Proposition for inverse transform method

- Let U be a UNIFORM (0,1) random variable
- If we define a random variable X with continuous distribution function F, then

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

• $F^{-1}(u)$ is defined as to equal that value of x for which



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Inverse transform method- Proof

Proof for inverse transform method

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

- Now, F(x) is a monotone function, it follows that $F^{-1}(U) \leq a$, iff $U \leq F(a)$
- $F_X(a) = P\{U \le F(a)\} == F(a)$
- Hence, we can simulate a RV X from continuos distribution FWhen F^{-1} is computable
 - by simulating a RV U, and then setting $X = F^{-1}(U)$



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Inverse transformation method

The rejection method Hazard rate method

Simulating an EXPONENTIAL RV

F(x)

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

- For $F(x) = 1 e^{-x}$,
- then $F^{-1}(u)$ is that value of x such that F(x) = u, i.e.

$$1 - e^{-x} = u$$
$$x = -\log(1 - u)$$



Simulating an EXPONENTIAL RV ...

F(x)

• Hence, if U is UNIFORM (0,1) variable, then following is a random variable EXPONENTIALLY distributed

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

- As 1 U is also UNIFORM on (0,1)
 - \bullet log U is EXPONENTIAL with mean 1
 - $-c \log U$ is EXPONENTIAL with mean c, as cX has mean c if X has mean 1



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The Rejection Method

- Suppose we have method for simulating an RV having density function g(x)
- ullet Using this basis, let's simulate from f(x)
- First, we simulate Y from g
- Then, ACCEPT this simulated value with a probability proportional to $\frac{f(Y)}{\sigma(Y)}$

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The Rejection Method ...

Technique for simulating from distribution f(x)

If

$$\frac{f(y)}{g(y)} \leqslant c$$
 for all y

Step_1 Simulate Y having density g(Y)

Step_2 Simulate *U*

Step_3 if
$$U \leqslant \frac{f(Y)}{cg(Y)}$$
, set $X = Y$; Otherwise RETURN to Step_1

Simulating a Normal RV

Simulating from Normal distribution

• A normal RV Z has mean (μ) = 0 and variance (σ^2) =1; absolute value of Z will have density-

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

• Given that X with $g(x) = e^{-x}$ is available

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

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Simulating from Normal distribution- procedure

- Generate independent random variables Y and U, Y being exponential with rate 1 and U being uniform on (0,1)
- ② If $U \le e^{-\frac{(x-1)^2}{2}}$, or equivalently, if $-\log U \ge \frac{(Y-1)^2}{2}$; set X = Y else return to 1.
- Having X, we can generate Z, by letting Z be equally likely to be either X or -X

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Hazard rate method

Simulatign an RV, S having hazard rate

- Let F be a CDF with $\bar{F}(0) = 1$
- let λ be hazaerd rate, given by $\lambda(t) = rac{f(t)}{\overline{F}(t)}$, t>0
- ullet That is, λ represents the instantaneous intensity
 - that an item having life distribution F will fail at time t given it has survived to that time

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- Let's simulate S having hazard rate function $\lambda(t)$
- To do so, let λ be such that

•
$$\lambda(t) \leq \lambda$$
 for all $t \geq 0$ & $\int_0^\infty \lambda(t) dt = \infty$

- Then, to simulate from $\lambda(t)$ we will
 - ullet simulate a Poisson process, with rate λ &
 - 'count' or 'accept' ONLY certain of these Poisson events

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 - COUNT an event that occurs at time t, independently of all else, with probability $\frac{\lambda(t)}{3}$

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Generating S having hazard rate

$$S: \lambda_S(t) = \lambda(t)$$

- Let $\lambda(t) \leq \lambda$ for all $t \geq 0$
- Generate pairs of RVs, U_i , X_i for $i \ge 1$; Where X_i being exponential with rate $\lambda \& U_i$ being uniform (0,1)
- STOP at

$$N = \min \left\{ n : U_n \le \frac{\lambda \left(\sum_{i=1}^n X_i\right)}{\lambda} \right\}$$

• Set $S = \sum_{i=1}^{N} X_i$

Generating S having hazard rate

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[Hazard rate method:] Definition

Stopping Time

Definition

An integer RV N, is said to be *stopping time* for the sequence X_1, X_2, \ldots , if the event $\{N = n\}$ is independent of X_{n+1}, X_{n+2}, \ldots for all $n = 1, 2, \ldots$

- Let X_n , n = 1, 2, ... be independent and such that $P\{X_n = 0\} = P\{X_n = 1\} = \frac{1}{2}$, n = 1, 2, ...
- If we let $N = \min\{n : X_1 + \dots + X_n = 10\}$
- Then, N is a stopping time
- e.g. N may be regarded as being the stopping time of EXPERIMENT that successively flips a fair coin and then stops when the number of HEADs reaches 10.

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- Then, *N* is a stopping time.
- e.g. *N* may be regarded as being the stopping time of EXPERIMENT that successively flips a fair coin and then stops when the number of HEADs reaches 10.

Simulating from discrete distributions

Simulating X having probability mass function Pj

- Let X be a discrete RV i.e. $P\{X=x_j\}=P_j$ for all $j=0,1\ldots$, where $\sum_i P_j=1$
- Inverse transform analogue; Let U be uniform (0,1)

Simulating from discrete distributions

Simulating X having probability mass function Pi

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Simulating X having probability mass function Pi

X can be set as following

$$X = \begin{cases} x_1 & \text{if} & U < P_1 \\ x_2 & \text{if} & P_1 < U < P_1 + P_2 \\ \vdots & & \\ x_j & \text{if} & \sum_{i=1}^{j-1} P_i < U < \sum_{i=1}^{j} P_i \\ \vdots & & \\ \vdots & & \end{cases}$$

As

$$P\{X = x_j\} = P\left\{\sum_{1}^{j-1} P_i < U < \sum_{1}^{j} P_i\right\} = P_j$$

Binomial Distribution Alias method

Simulating from discrete distributions ...

Determining optimal number of runs

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Simulating from Geometric distribution

Simulating X having GEOMETRIC probability mass function

ullet Let's simulate X having Geometric pmf, i.e.

$$P\{X=i\} = p(1-p)^{i-1}$$

$$\sum_{i=1}^{j-1} P\{X=i\} = 1 - P\{X > j-1\} = 1 - (1-p)^{i-1}$$

 We start with generating U, and then setting X to that value of j for which

$$1 - (1 - p)^{i-1} < U < 1 - (1 - p)^{i}$$
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Simulating from Geometric distribution ...

Simulating X having GEOMETRIC probability mass function

• As U has same distribution as 1-U, X can also be defined as

$$X = \min \left\{ j : (1-p)^j < U \right\} = \min \left\{ j : j > \frac{\log U}{\log (1-p)} \right\}$$
$$= 1 + \frac{\log U}{\log (1-p)}$$

Simulating a Binomial RV

Binomial discrete RV

- A binomial RV (n, p) can be most easily simulated considering that
 - \bullet it can be expressed as the sum of n independent Bernoulli RV
- e.g., if $U_1, U_2, \dots U_n$ are independent Uniform (0,1) RVs ther letting

$$X_i = \left\{ \begin{array}{ll} 1 & \text{if } U_i$$

• then $X = \sum_{i=1}^{n} X_i$ is a binomial RV with (n, p)



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Simulating a Binomial RV: Procedure

Improvements

- <1->The previous method requires generation of *n* random numbers
- <2->Instead of using value of *U*, the previous algorithm uses the fact *U_i* < *p* or not
- <3->Conditional distribution of *U* given that *U* < *p* is uniform in (0,*p*)
 & conditional distribution of *U* given that *U* > *p* is uniform in (*p*,1)

Procedure

Step_1 Let
$$\alpha = 1/p$$
 and $\beta = 1/(1-p)$

Step 2 Set
$$k = 0$$

Step_3 Generate a uniform RV
$$\it U$$

Step_4 If
$$k = n$$
 stop, else RESET $k = k + 1$

Step_5 If
$$U \le p$$
 set $X_k = 1$ and RESET U to αU . If $U > p$ set $X_k = 0$ and RESET U to $\beta(U - p)$. RETURN to Step 4

Outline

- Introduction
 - What is Monte Carlo simulation?
- Quantum General techniques for simulating continuous RVs
 - Inverse transformation method
 - The rejection method
 - Hazard rate method
- 3 Special techniques for simulating continuous RVs
- 4 Simulating from discrete distributions
 - Alias method
- Multivariate distributions & Stochastic Processes
- 6 Variance reduction techniques
- Determining optimal number of runs



Alias Method

- Let quantities, $P, P^{(k)}, Q^{(k)}, k \le n-1$ represent pmf on 1, 2, ..., n i.e. they are n-vectors of non-negative numbers summing to 1
- Additionally, each of $P^{(k)}$ will have at most k non-zero components
- Each of $\mathbf{Q}^{(k)}$ will have at most 2 non-zero components

Let $P = \{P_i, i = 1, 2, ..., n\}$ denote pmf, then (a) there exists and i, $1 \le i \le n$, such that $P_i < \frac{1}{n-1}$, and (b) for this i, there exists a $j, j \ne i$, such that $P_i + P_j \ge \frac{1}{n-1}$

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Corollary

Let $P = \{P_i, i = 1, 2, ..., n\}$ denote pmf, then

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Alias Method ...

Alias Method ...

• Any pmf **P** can be represented as an equally weighted mixture of n-1 pmf **Q**, i.e. for suitably defined $Q^{(1)}, Q^{(2)}, \dots Q^{(n-1)}$

$$P = \frac{1}{n-1} \sum_{k=1}^{n-1} Q^{(k)}$$

• Alongwith example illustration, a general technique is described

Example- Alias method ... (1)

Example: Alias Method ...

- Let $P_1 = \frac{7}{16}, P_2 = \frac{1}{2}, P_3 = \frac{1}{16}$ stand for **P**. here n = 3 and hence k = 1, 2
- lets' presume following two 2-point mass-functions $Q^{(1)} \& Q^{(2)}$ to constitute P.
 - $Q^{(1)}$: all weight on 3 and 2
 - $Q^{(2)}$: may be derived using $Q^{(1)}$ and

$$P_j = \frac{1}{2} \left(Q_j^{(1)} + Q_j^{(2)} \right) \ j = 1, 2, 3$$

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Example: Alias Method ...

•
$$\Rightarrow Q_3^{(2)} = 0$$
; and

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$$Q_3^{(1)} = 2P_3$$
; $Q_2^{(1)} = 1 - Q_3^{(1)} = \frac{1}{8}$; $Q_1^{(1)} = 0$

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• Similar procedure may be followed for case of 4-point mass-function P: n = 4, k = 3



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Alias Method: General rocedure

General procedure: Alias Method

 This method outlines proceure for any n-point pmf P can be written as follows; We presume corollary/Lemma above for i and j;

$$P = \frac{1}{n-1} \sum_{k=1}^{n-1} Q^{(k)}$$

- ullet Lets define $Q^{(1)}$ concentrating on points i and j
 - which will contain all of the mass for point i by noting that in representtion above, $Q_i^{(k)} = 0$ for k = 2, 3, ..., n-1
 - i.e. $Q_i^{(1)} = (n-1)P_i$ and so $Q_j^{(1)} = 1 (n-1)P_i$



Alias Method: General rocedure ... (2)

General procedure: Alias Method

Writing

$$P = \frac{1}{n-1}Q^{(1)} + \frac{n-2}{n-1}P^{(n-1)}$$

• here, $P^{(n-1)}$ represents the remaining mass, hence

•

$$\begin{array}{lcl} P_i^{(n-1)} & = & 0 \\ P_j^{(n-1)} & = & \frac{n-1}{n-2} \left(P_j - \frac{1}{n-1} Q_j^{(1)} \right) = \frac{n-1}{n-2} \left(P_i + P_j - \frac{1}{n-1} \right) \\ P_k^{(n-1)} & = & \frac{n-1}{n-2} P_k, \quad k \neq i \text{ or } j \end{array}$$

Alias Method: General rocedure ... (3)

General procedure: Alias Method

• Repeating to expand $P^{(n-1)}$ likewise

$$\mathbf{P}^{(n-1)} = \frac{1}{n-2}Q^{(2)} + \frac{n-3}{n-2}\mathbf{P}^{(n-2)}$$

Hence, full expansion,

$$\mathbf{P} = \frac{1}{n-1}Q^{(1)} + \frac{1}{n-1}Q^{(2)} + \frac{n-3}{n-2}\mathbf{P}^{(n-2)}$$

$$P = \frac{1}{n-1} \left(Q^{(1)} + Q^{(2)} + \ldots + Q^{(n-1)} \right)$$



Algorithm for Alias method

Algorithm

The P can now be simulated as follows

- Generating random integer N equally likely to be either 1, 2, ... (n-1)
- If N is such that $Q^{(N)}$ puts positive weight only on point i_N and j_N ,
 - then we can set X equal to i_N , if second random number is less that $Q_{i_N}^{(N)}$; equal to j_N , otherwise,
 - Step_1 Generate U_1 and set $N = 1 + [(n-1)U_1]$ Step_2 Generate U_2 and set

$$X = \left\{ \begin{array}{ll} i_N & \textit{if } U_2 < Q_{i_{\pmb{N}}}^{(N)} \\ j_N & \textit{Otherwise} \end{array} \right.$$

Error minimization

Minimizing error while generating X

- Let $X_1, X_2, ..., X_n$ have given distribution,
 - having density function $f(x_1, x_2, ..., x_n)$
- ullet Objective is to find the expected value of E[g(X)]
 - $\bullet \ \theta = E\left[g\left(X_1, X_2, \dots X_n\right)\right]$

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$$Y^{(2)} = g\left(X_1^{(2)}, X_2^{(2)}, \dots X_n^{(2)}\right)$$

•
$$\bar{Y} = \sum_{i=1}^{k} Y_i / k$$
 and $E[\bar{Y}] = \theta$, $E[(\bar{Y} - \theta)^2] = Var(\bar{Y})$

• \overline{Y} is an estimator of θ ; we wish to minimize $E\left[\left(\overline{Y}-\theta\right)^2\right]$

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Use of Anti-thetic variables

Let Y_1 and Y_2 be idetically distributed RVs, with mean θ

$$Var\left(\frac{Y_{1} + Y_{2}}{2}\right) = \frac{1}{4}(Var(Y_{1}) + Var(Y_{1}) + 2Cov(Y_{1}, Y_{2}))$$
$$= \frac{Var(Y_{1})}{2} + \frac{Cov(Y_{1}, Y_{2})}{2}$$

Variance reduction- Using Antithetic variables

- It would be more advantageous for Y_1 and Y_2 NOT to be idetically distributed, BUT negatively correlated
- $X_1, X_2, ..., X_n$ are independent and simulated by inverse method from U
 - X_i is simulated from $F_i^{-1}(U)$

Determining optimal number of runs

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$$Y_1 = g(F_1^{-1}(U_1), F_2^{-1}(U_2), \dots F^{-n}(U_n))$$

• Since, 91 - U) is also uniform (0,1) and is negatively correlated with U

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$$Y_2 = g(F_1^{-1}(1-U_1), F_2^{-1}(1-U_2), \dots F^{-n}(1-U_n))$$

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Number of RUNs

- Let use simulation to generate i.i.d. (independent idetically distributed) $Y_1, Y_2, ..., Y_r$ having mean μ and variance σ^2
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 - BUT σ^2 is not known in advance
- To get around this, we initially simulate k times to evaluate σ^2 , and use simulated $Y^{(1)}, Y^{(2)}, \dots Y^{(k)}$ to estimate σ^2 by sample variance

$$\sum \frac{\left(Y^{(k)} - \overline{Y}_k\right)^2}{k - 1}$$

 Based on this estimate, rest of the r – k values can be simulated

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Introduction
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Simulating from discrete distributions
Multivariate distributions & Stochastic Processes
Variance reduction techniques
Determining optimal number of runs

Completed!

END

Thanks!