STAT 380 Lecture 10

Simulation

Monte Carlo computation of expected value:

To compute $\mathrm{E}(X)$: do experiment n times to generate n independent observations all with same distribution as X.

Get $X_1, \ldots, X_n$.

Use

$$\bar{X} = \frac{1}{n}\sum_1^n X_i$$

as an estimate of $\mathrm{E}(X)$

To estimate $\mathrm{E}(g(X))$: use same X_i and compute

$$\frac{1}{n}\sum_1^n g(X_i)\,.$$

Random Number Generation

In practice: random quantities are not used.

Use: **pseudo-random** uniform random numbers.

They "behave like" iid Uniform(0,1) variables.

Many, many generators. One standard kind: **linear congruential generators**.

Start with x_0 an integer in range $0 \le x_0 < m$. Compute

$$x_{n+1} = ax_n + b \mod m$$

Here the **mod** means compute the remainder after division by m.

Integers a and b are chosen so that

- the sequence $x_0, \ldots, x_{m-1}$ runs through the set $\{0, \ldots, m-1\}$ (or as much of it is possible, sometimes).

- the sequence of pairs

  $$(x_0, x_1), (x_1, x_2), \ldots, (x_{m-1}, x_m)$$

  fills up as much of the square $\{(i, j) : 1 \le i, j \le m-1\}$.

- similarly for triples (x_k, x_{k+1}, x_{k+2}).

Use

$$U_n = \frac{x_n}{m}$$

as Uniform(0,1) random numbers.

General Random Variables

We now pretend we can generate $U_1, U_2, \ldots$ which are iid Uniform(0,1). Monte Carlo methods for generating a sample:

- Transformation:
  - Inverse Probability Integral Transform
  - Multivariate (e.g. Box Müller)
- Acceptance Rejection
- Markov Chain Monte Carlo

Inverse (Probability Integral) Transform

Fact: F continuous CDF and X, U satisfy

$$U = F(X)$$

then U ~Uniform(0,1) if and only if $X \sim F$.

Proof: For simplicity: assume F strictly increasing on inverval (a, b) with $F(b) = 1$ and $F(a) = 0$.

If U ~Uniform(0,1) then

$$\begin{aligned} P(X \le x) &= P(F(X) \le F(x)) \\ &= P(U \le F(x)) \\ &= F(x) \end{aligned}$$

Conversely: if $X \sim F$ and $0 < u < 1$ then there is a unique x such that $F(x) = u$

$$\begin{aligned} P(U \le u) &= P(F(X) \le F(x)) \\ &= P(X \le x) \\ &= F(x) \\ &= u \end{aligned}$$

Application: generate U and solve $F(X) = U$ for X to get $X = F^{-1}(U)$ which has cdf F.

Example:For the exponential distribution

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

Set $F(X) = U$ and solve to get

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

Observation: $U \sim 1 - U$ so $X = -\log(U)/\lambda$ also has an Exponential(λ) distribution.

Example:: for F the standard normal cdf solving

$$F(X) = U$$

requires numerical approximation but such solutions are built in to many languages.

Special purpose transformations:

Example:: If X and Y are iid $N(0, 1)$ define $R \geq 0$ and $\Theta \in [0, 2\pi)$ by

$$X = R\cos(\Theta) \qquad Y = R\sin(\Theta)$$

NOTE: Book says

$$\Theta = \tan^{-1}(Y/X)$$

but this takes values in $(-\pi/2, \pi/2)$; notation

$$\tan^{-1}(x, y)$$

means angle θ in $[0, 2\pi)$ so that

$$\frac{x}{\sqrt{x^2 + y^2}} = \cos(\theta) \qquad \frac{y}{\sqrt{x^2 + y^2}} = \sin(\theta)\,.$$

Then

$$\{(r, \theta) : r \leq r^*, \theta \leq \theta^*\}$$

is part of circle of radius r^*. (Start at $(r^*, 0)$ and go clockwise to angle θ^*.)

Compute joint cdf of R, Θ at r^*, θ^*.

Define

$$C = \{(x,y) : x^2 + y^2 \le (r^*)^2,$$
$$0 \le \tan^{-1}(x,y) \le \theta^*\}$$

Then

$$P(R \le r, \Theta \le \theta)$$
$$= \iint_C \frac{e^{-(x^2+y^2)/2}}{2\pi} dxdy$$

Do integral in polar co-ordinates to get

$$\int_0^{r^*} \int_0^{\theta^*} \frac{e^{-r^2/2}}{2\pi} r dr d\theta$$

The θ integral just gives

$$\theta^*/(2\pi)$$

The r integral then gives

$$1 - e^{-(r^*)^2/2}$$

So

$$P(R \le r^*, \Theta \le \theta^*) = \left(1 - e^{-(r^*)^2/2}\right) \times \frac{\theta^*}{2\pi}$$

Product of two cdfs so: R and Θ are independent.

Moreover R^2 has cdf

$$P(R^2 \le x) = 1 - e^{-x/2}$$

which is Exponential with rate 1/2.

Θ is Uniform$(0, 2\pi)$.

So: generate U_1, U_2 iid Uniform(0,1).

Define

$$\Theta = 2\pi U_2$$

and

$$R = \sqrt{-2\log(U_1)}$$

Put

$$X = R\cos(\Theta) \qquad Y = R\sin(\Theta)$$

You have generated two independent $N(0,1)$ variables.

Acceptance Rejection

If $F(X) = U$ difficult to solve (eg F hard to compute) sometimes use acceptance rejection.

Goal: generate $X \sim F$ where $F' = f$.

Tactic: find density g and constant c such that

$$f(x) \leq cg(x)$$

and s.t. can generate Y from density g.

Algorithm:

1. Generate Y which has density g.
2. Generate $U \sim$Uniform(0,1) independent of Y.
3. If $U \leq f(Y)/\{cg(Y)\}$ let $X = Y$.
4. If not reject Y and go back to step 1; repeat, generating new Y and U (independently) till you accept a Y.

Facts:

- Since you repeat the same experiment each trial: number of trials, N, success is Geometric (and sure to be finite).
- The probability of success on a individual trial is

$$\begin{aligned} P[U \leq f(Y)/\{cg(Y)\}] \\ &= \int P[U \leq f(y)/\{cg(y)\}|Y = y]g(y)dy \\ &= \int \frac{f(y)}{cg(y)}g(y)dy \\ &= \frac{1}{c}\int f(y)dy \\ &= 1/c \end{aligned}$$

so

$$\mathrm{E}(N) = 1/c$$

Most important fact: $X \sim f$:

Proof: this is like the old craps example:

We compute

$$P(X \le x) = P[Y \le x | U \le f(Y)/\{cg(Y)\}]$$

(condition on the first iteration where the condition is met).

Condition on Y to get

$$\begin{aligned} & P(X \le x) \\ & = \frac{\int_{-\infty}^x P[U \le f(Y)/\{cg(Y)\}|Y = y]g(y)dy}{P[U \le f(Y)/\{cg(Y)\}]} \\ & = \frac{\int_{-\infty}^x \frac{f(y)}{cg(y)} g(y)dy}{1/c} \\ & = \int_{-\infty}^x f(y)dy \\ & = F(x) \end{aligned}$$

as desired.

Example:Half normal distribution: X has density

$$f(x) = \frac{2e^{-x^2/2}}{\sqrt{2\pi}} 1(x > 0)$$

(Density of absolute value of $N(0,1)$.)

Use $g(x) = ae^{-ax}1(x > 0$. To find c maximize

$$\frac{f(x)}{g(x)} = \frac{e^{-x^2/2+ax}}{a\sqrt{2\pi}}$$

Rewrite as

$$\frac{e^{a^2/2}e^{-(x-a)^2/2}}{a\sqrt{2\pi}}$$

Maximum is at $x = a$ giving

$$c = \frac{e^{a^2/2}}{a\sqrt{2\pi}}$$

Choose a to minimize c (or $\log(c)$); get $a = 1$ so

$$c = \frac{e}{\sqrt{2\pi}}$$

Algorithm is then: generate $Y = -\log(U_1)$ and then compute

$$e^{-(Y-1)^2}$$

Generate U_2 and if

$$U_2 \leq e^{-(Y-1)^2}$$

accept Y otherwise try again.

To generate $N(0,1)$: use a third U to pick a sign at random: negative if $u < 1/2$ otherwise positive.

Discrete Distributions

The inverse transformation method works for discrete distributions.

X has possible values $\{x_1, x_2, \ldots\}$ with probabilities $\{p_1, p_2, \ldots\}$ compute cumulative probabilities

$$P_k = p_1 + \cdots + p_k$$

with $P_0 = 0$.

Generate $U \sim$Uniform(0,1).

Find k such that

$$P_{k-1} < U \leq P_k$$

Put $X = x_k$.