Lecture Notes to Accompany

Scientific Computing

An Introductory Survey Second Edition

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Chapter 13

Random Numbers and Stochastic Simulation

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Stochastic Simulation

Stochastic simulation methods mimic or replicate behavior of system by exploiting randomness to obtain statistical sample of possible outcomes

Because of randomness involved, simulation methods are also known as Monte Carlo methods ods

Such methods are useful for studying:

- Nondeterministic (stochastic) processes
- Deterministic systems that are too complicated to model analytically
- Deterministic problems whose high dimensionality makes standard discretizations infeasible (e.g., Monte Carlo integration)

Stochastic Simulation, continued

Two main requirements for using stochastic simulation methods:

- Knowledge of relevant probability distributions
- Supply of random numbers for making random choices

Knowledge of relevant probability distributions depends on theoretical or empirical information about physical system being simulated

By simulating large number of trials, probability distribution of overall results can be approximated, with accuracy attained depending on number of trials

Randomness

Randomness is somewhat difficult to define, but we usually associate randomness with unpredictability

One definition is that sequence of numbers is *random* if it has no shorter description than itself

Physical processes, such as flipping coin or tossing dice, are deterministic if enough is known about equations governing their motion and appropriate initial conditions

Even for deterministic systems, extreme sensitivity to initial conditions can make their chaotic behavior unpredictable in practice

Deterministic or not, highly complicated systems are often tractable only by stochastic simulation methods

Repeatability

In addition to unpredictability, another distinguishing characteristic of true randomness is lack of *repeatability*

However, lack of repeatability could make testing algorithms or debugging computer programs difficult, if not impossible

Repeatability is desirable in this sense, but one must take care to ensure that independence is maintained among trials

Pseudorandom Numbers

Although random numbers were once supplied by physical processes or tables, they are now produced by computers

Computer algorithms for generating random numbers are in fact deterministic, although sequence generated may *appear* random in that it exhibits no apparent pattern

Such sequences of numbers are more accurately called *pseudorandom*

Although pseudorandom sequence may appear random, it is in fact quite predictable and reproducible, which is important for debugging and verifying results

Because only finite number of numbers can be represented in computer, any sequence must eventually repeat

Random Number Generators

A good random number generator should have as many of following properties as possible

- *Random pattern*: passes statistical tests of randomness
- Long period: goes as long as possible before repeating
- *Efficiency*: executes rapidly and requires little storage
- *Repeatability*: produces same sequence if started with same initial conditions
- Portability: runs on different kinds of computers and is capable of producing same sequence on each

Random Number Generators, cont.

Early attempts at producing random number generators on computers often relied on very complicated procedures, whose very complexity was felt to ensure randomness

Example is "midsquare" method, which squares each member of sequence and takes middle portion of result as next member of sequence

Lack of theoretical understanding of such methods proved disastrous, and it was soon recognized that simple methods with well-understood theoretical basis are far preferable

Congruential Generators

Congruential random number generators have form

$$x_k = (ax_{k-1} + c) (\operatorname{mod} M),$$

where a and c are given integers

Starting integer x_0 is called *seed*

Integer M is approximately (often equal to) largest integer representable on machine

Quality of such generator depends on choices of a and c, and in any case its period cannot exceed M

Congruential Generators, cont.

It is possible to obtain reasonably good random number generator using this method, but values of a and c must be chosen *very* carefully

Many system-supplied random number generators are of congruential type, and some of them are notoriously poor

Congruential generator produces random integers between 0 and ${\cal M}$

To produce random floating-point numbers, say uniformly distributed on interval [0, 1), random integers must be divided by M

Fibonacci Generators

Alternative methods that produce floating-point random numbers on interval [0, 1) directly are Fibonacci generators, which generate new value as difference, sum, or product of previous values

Typical example is subtractive generator

$$x_k = x_{k-17} - x_{k-5}$$

This generator has *lags* of 17 and 5

Lags must be chosen carefully to produce good subtractive generator

Such formula may produce negative result, in which case remedy is to add 1 to get back into interval [0, 1)

Fibonacci Generators, cont.

Fibonacci generators require more storage than congruential generator, and also require special procedure to get started

Fibonacci generators require no division to produce floating-point results

Well-designed Fibonacci generators have very good statistical properties

Fibonacci generators can have much longer period than congruential generators, since repetition of one member of sequence does not entail that all subsequent members will also repeat in same order

Sampling on Other Intervals

If we need uniform distribution on some other interval [a, b), then we can modify values x_k generated on [0, 1) by transformation

$$(b-a)x_k + a$$

to obtain random numbers that are uniformly distributed on desired interval

Nonuniform Distributions

More difficult problem is to sample from nonuniform distributions

If cumulative distribution function of desired probability density function is easily invertible, then we can generate random samples with desired distribution by generating uniform random numbers and inverting them

For example, to sample from exponential distribution

$$f(t) = \lambda e^{-\lambda t}, \quad t > 0,$$

we can take

$$x_k = -\log(1 - y_k)/\lambda,$$

where y_k is uniform on [0, 1)

Unfortunately, many important distributions are not easily invertible, and special methods must be employed to generate random numbers efficiently for these distributions

Normal Distribution

Important example is generation of random numbers that are normally distributed with given mean and variance

Available routines often assume mean of 0 and variance of 1

If some other mean μ and variance σ^2 are desired, then each value x_k produced by routine can be modified by transformation $\sigma x_k + \mu$ to achieve desired normal distribution

Quasi-Random Sequences

For some applications, achieving reasonably uniform coverage of sampled volume can be more important than whether sample points are truly random

Truly random sequences tend to exhibit random clumping, leading to uneven coverage of sampled volume for given number of points

Perfectly uniform coverage can be achieved by using regular grid of sample points, but this approach does not scale well to higher dimensions

Compromise between these extremes of coverage and randomness is provided by *quasirandom sequences*

Quasi-Random Sequences, cont.

Such sequences are not random at all but are carefully constructed to give uniform coverage of sampled volume while maintaining reasonably random appearance

By design, points tend to avoid each other, so clumping associated with true randomness is eliminated

