Malvin H. Kalos, Paula A. Whitlock

Monte Carlo Methods

Related Titles

J.S. Dagpunar

Simulation and Monte Carlo

With applications in finance and MCMC

2007
ISBN: 978-0-470-85494-5

B.D. Ripley

Stochastic Simulation

2000
ISBN: 978-0-470-00960-4

A. Korngold

Leveraging Good Will – Strengthening Nonprofits by Engaging Businesses

2005. E-Book
ISBN: 978-0-7879-8188-4

A. Dubi

Monte Carlo Applications in Systems Engineering

2000
ISBN: 978-0-471-98172-5

R.H. Landau, M.J. Páez

Computational Physics

Problem Solving with Computers

1997
ISBN: 978-0-471-11590-8

Malvin H. Kalos, Paula A. Whitlock

Monte Carlo Methods

Second Revised and Enlarged Edition

WILEY-VCH Verlag GmbH & Co. KGaA

The Authors

Dr. Malvin H. Kalos
Lawrence Livermore National Laboratory
Livermore, USA

Dr. Paula A. Whitlock
CIS Department
Brooklyn College
Brooklyn, USA

Cover Illustration

Heather Marvin, Jonathan Stuart-Moore,
Shodor Education Foundation

Library of Congress Card No.: applied for

British Library Cataloguing-in-Publication Data
A catalogue record for this book is available from the British Library.

Bibliographic information published by the Deutsche Nationalbibliothek
Die Deutsche Nationalbibliothek lists this publication in the Deutsche National-bibliografie; detailed bibliographic data are available in the Internet at http://dnb.d-nb.de

Typesetting Laserwords Private Ltd, Chennai, India
Printing betz-druck GmbH, Darmstadt
Bookbinding Litges & Dopf GmbH, Heppenheim

Printed in the Federal Republic of Germany
Printed on acid-free paper

ISBN: 978-3-527-40760-6

Contents

Monte Carlo Methods. Second Edition. M.H. Kalos and P.A. Whitlock

ISBN: 978-3-527-40760-6

Preface to the Second Edition

We began our preface to the first edition with the sentence, ''This book has had a long gestation period.'' The gestation of our second edition has been equally long.

In a sense, more has changed in the last twenty-two years in the theory and practice of Monte Carlo methods than in the twenty-two years before that. Tremendous strides have been made in the development of new techniques and applications. This is of course primarily a testament to the power of the methods and the breadth of their applicability, but it is also a testament to the breathtaking evolution of computing power which has made possible much wider and deeper experimentation and studies. More computing power enables more challenging applications, which exposes the need for more effective methods. In particular, the appearance of massively parallel computers – with as many as 200 000 processors – and for which many Monte Carlo calculations are well suited, has accelerated the evolution.

We have also seen new fields – such as financial computing – for which Monte Carlo methods are an essential tool.

As with almost all intellectual efforts, the synergy between widespread applicability and widespread interest has produced an exponential growth in new ideas.

It seemed to us that the aims of our previous edition – to give a short but unified approach to the field, limiting ourselves to applications in the physical sciences – is needed now as much, or perhaps more than before. We have corrected, revised, and extended the material in the first edition, and we have added new material on various quantum MC techniques, on Brownian motion, Poisson processes, simulated annealing, adaptive MC, and on quasi-MC.

As always, we have benefited from the collaboration and advice of many people. Our decades of friendship and research with Geoffrey Chester were essential and inspirational. We have continued to learn much from David Ceperley and Kevin Schmidt. In more recent times, MHK has had the privilege of working with Vasily Bulatov, Jaime Marian and Enrique Martinez,

Monte Carlo Methods. Second Edition. M.H. Kalos and P.A. Whitlock

ISBN: 978-3-527-40760-6

and long term interactions with Francesco Pederiva and Randolph Hood. PAW has enjoyed working with Marvin Bishop, Silvio Vitiello and Todor Gurov.

New York, July 2008

Malvin H. Kalos
Paula A. Whitlock

Preface to the First Edition

This book has had a long gestation period. While it simmered on the back burner, we pursued research in various aspects of Monte Carlo methods and their application to the simulation of physical systems. Out of this diversity we believe we see a basic way of looking at the field. It is unfortunate that some observers and even some specialists of Monte Carlo methods seem to regard Monte Carlo as a bag of miscellaneous devices. Often it comes across that way when applied. It is true that like many other technical endeavors, especially those with as intensely practical an outlook as Monte Carlo methods, a body of ingenious tricks has arisen, awaiting invocation as needed. But we believe – and hope that our book is successful in conveying both in a general and a practical sense – that there are a number of unifying ideas that underlie the study and use of good Monte Carlo methods.

The first is the importance of random walks – on the one hand as they occur in natural stochastic systems, and on the other, in their relation to integral and differential equations.

The other basic theme is that of variance reduction and, above all, of importance sampling as a technical means of achieving variance reduction. Importance sampling is the transformation of a basically straight-forward random sampling method by changing variables or, what amounts to the same thing, by changing the underlying probability distribution while leaving a required mean unchanged. It is by no means the only method, nor in particular cases the best method, for variance reduction. But it offers a coherent point of view about variance reduction. In important cases it offers the theoretical possibility of zero variance. The use of approximations to variance minimizing transformations is a powerful technique for the introduction of a priori knowledge based on experience or approximate solution of the problem at hand into a still exact numerical treatment based on Monte Carlo methods.

We believe that these ideas have stood us well in our research in radiation transport, in statistical physics, and in quantum mechanics and have served to unify them intellectually. We offer them to our readers in the hope that our point of view will make the theory and practice of Monte Carlo more interesting and more effective.

Monte Carlo Methods. Second Edition. M.H. Kalos and P.A. Whitlock

ISBN: 978-3-527-40760-6

This book is a distillation of some years of practice and thought about Monte Carlo methods. As such it has benefited from the ideas and suggestions of many friends and colleagues, too numerous to list in full. It would be remiss not to mention some of them, however, starting with Gerald Goertzel, who first introduced one of us (MHK) to the mixed joys of Monte Carlo on primitive computers, and to many of the basic ideas expressed in our book. Others from whom we have learned include particularly Harry Soodak, Eugene Troubetzkoy, Herbert Steinberg, Loup Verlet, Robert Coveyou, Phillip Mittleman, Herbert Goldstein, David Ceperley, Kevin Schmidt, and Geoffrey Chester. Notes of early lectures taken by Jacob Celnik were very helpful.

We gratefully acknowledge the help and encouragement of our many colleagues and students during the time this book was being written. We especially thank David Ceperley for giving the original lecture on which Chapter 5 was based. Youqin Zhong and John Halton gave numerous suggestions for improving earlier versions of the manuscript. We thank them for their efforts and hope the final book lives up to their expectations.

New York, August 1986

Malvin H. Kalos
Paula A. Whitlock

1
What is Monte Carlo?

1.1
Introduction

The name *Monte Carlo* was applied to a class of mathematical methods first used by scientists working on the development of nuclear weapons in Los Alamos in the 1940s. The essence of the method is the invention of games of chance whose behavior and outcome can be used to study some interesting phenomena. While there is no essential link to computers, the effectiveness of numerical or simulated gambling as a serious scientific pursuit is enormously enhanced by the availability of modern digital computers.

It is interesting, and may strike some as remarkable, that carrying out games of chance or random sampling will produce anything worthwhile. Indeed, some authors have claimed that Monte Carlo will never be a method of choice for other than rough estimates of numerical quantities.

Before asserting the contrary, we shall give a few examples of what we mean and do not mean by Monte Carlo calculations. Consider a circle and its circumscribed square. The ratio of the area of the circle to the area of the square is $\pi/4$. It is plausible that if points were placed at random in the square, the fraction $\pi/4$ would also lie inside the circle. If that is true (and we shall prove later that in a certain sense it is), then one could measure $\pi l4$ by putting a round cake pan with diameter L inside a square cake pan with side L and collecting rain in both. It is also possible to program a computer to generate random pairs of Cartesian coordinates to represent random points in the square and count the fraction that lies in the circle. This fraction as determined from many experiments should be close to $\pi/4$, and the fraction would be called an *estimate for* $\pi/4$. In 1 000 000 experiments, it is very likely (95% chance) that the number of points inside the circle would range between 784 600 and 786 200, yielding estimates of $\pi/4$ that are between 0.7846 and 0.7862, compared with the true value of 0.785398.

The example illustrates that random sampling may be used to solve a mathematical problem, in this case, evaluation of a definite integral,

$$I = \int_0^1 \int_0^{\sqrt{1-x^2}} \mathrm{d}x\, \mathrm{d}y. \tag{1.1}$$

Monte Carlo Methods. Second Edition. M.H. Kalos and P.A. Whitlock

ISBN: 978-3-527-40760-6

The answers obtained by the above procedure are statistical in nature and subject to the laws of chance. This aspect of Monte Carlo is a drawback, but not a fatal one, since one can determine how accurate the answer is, and obtain a more accurate answer, if needed, by conducting more experiments. Sometimes, in spite of the random character of the answer, it is the most accurate answer that can be obtained for a given investment of computer time. The determination of the value of π can of course be done faster and more accurately by non–Monte Carlo methods. In many dimensions, however, Monte Carlo methods are often the only effective means of evaluating integrals.

A second and complementary example of a Monte Carlo calculation is one that Ulam [1] cited in his autobiography. Suppose one wished to estimate the chances of winning at solitaire, assuming the deck is perfectly shuffled before laying out the cards. Once we have chosen a particular strategy for placing one pile of cards on another, the problem is a straightforward one in elementary probability theory, but is also a very tedious one. It would not be difficult to program a computer to randomize lists representing the 52 cards of a deck, prepare lists representing the different piles, and then simulate the playing of the game to completion. Observation over many repetitions would lead to a Monte Carlo estimate of the chance of success. This method would in fact be the easiest way of making any such estimate. We can regard the computer gambling as a faithful simulation of the real random process, namely, the card shuffling.

Nowadays, random numbers are used in many ways associated with computers. These include, for example, computer games and generation of synthetic data for testing. These are of course interesting, but not what we consider Monte Carlos, since they do not produce numerical results. A definition of a Monte Carlo method would be one that involves deliberate use of random numbers in a calculation that has the structure of a stochastic process. By *stochastic process*, we mean a sequence of states whose evolution is determined by random events. In a computer, these are generated by a deterministic algorithm that generates a sequence of pseudorandom numbers, which mimics the properties of truly random numbers.

A distinction is sometimes made between simulation and Monte Carlo. In this view, simulation is a rather direct transcription into computing terms of a natural stochastic process (as in the example of solitaire). Monte Carlo, by contrast, is the solution by probabilistic methods of nonprobabilistic problems (as in the example of π). The distinction is somewhat useful, but often impossible to maintain. The emission of radiation from atoms and its interaction with matter is an example of a natural stochastic process, since each event is to some degree unpredictable (Chapter 6). It lends itself very well to a rather straightforward stochastic simulation, but the average behavior of such radiations can also be described by mathematical equations whose numerical solution can be obtained using Monte Carlo methods. Indeed, the same computer code can be viewed simultaneously as a ''natural simulation'' or as a solution of the equations by random sampling. As we shall also see, the latter point of view

is essential in formulating efficient schemes. The main point we wish to stress here is that the same techniques directly yield both powerful and expressive simulation and powerful and efficient numerical methods for a wide class of problems.

We would like to return to the issue of whether Monte Carlo calculations are in fact worth carrying out. This can be answered in a very pragmatic way: many people use them and they have become an accepted part of scientific practice in many fields. The reasons do not always depend on pure computational economy. As in our solitaire example, convenience, ease, directness, and expressiveness of the method are important assets–increasingly so as pure computational power becomes cheaper. In addition, as asserted in discussing π, Monte Carlo methods are in fact computationally effective, compared with deterministic methods when treating many-dimensional problems. That is why partly their use is so widespread in operations research, in radiation transport (where problems up to seven dimensions must be dealt with), and especially in statistical physics and chemistry (where systems of thousands of particles can now be treated quite routinely). An exciting development in the past few years is the use of Monte Carlo methods to evaluate path integrals associated with field theories as in quantum chromodynamics.

1.2
Topics to be Covered

This book focuses on several major areas. The first topic addressed is a review of some simple probability ideas with emphasis on concepts central to Monte Carlo theory. For more rigorous information on probability theory, references to standard texts are given. Further chapters deal with the crucial question of how random events (or reasonable facsimiles) are programmed on a computer. Techniques for sampling complicated distributions are necessary for applications and, equally important, serve as a basis for illustrating the concepts of probability theory that are used throughout.

Then we consider quadratures in finite-dimensional spaces. Attention is paid to the important and interesting case of singular integrands, especially those for which the variance of a straightforward estimate does not exist so that the usual central limit theorems do not apply. These are cases for which variance reduction methods have an immediate and direct payoff. Also explored are quasi-Monte Carlo methods, which use low-discrepancy sequences that uniformly fill the multidimensional space.

Finally, applications of Monte Carlo methods are discussed. An introduction to current uses in statistical physics is given. The simulation of a simple example of radiation transport is developed, and this naturally leads to the solution of integral equations by Monte Carlo. The ideas are then used as a framework upon which a relationship between random walks and integral equations could be constructed and also to introduce the fundamentals of variance reduction for the simulation of random walks.

1.3 A Short History of Monte Carlo

Perhaps the earliest documented use of random sampling to find the solution to an integral is that of Comte de Buffon [2]. In 1777, he described the following experiment. A needle of length L is thrown at random onto a horizontal plane ruled with straight lines a distance $d(d > L)$ apart. What is the probability, P, that the needle will intersect one of these lines? Comte de Buffon performed the experiment of throwing the needle many times to determine P. He also carried out the mathematical analysis of the problem and showed that

$$P = \frac{2L}{\pi d}. \tag{1.2}$$

Some years later, Laplace [3] suggested that this idea could be used to evaluate π from throws of the needle. This is indeed a Monte Carlo determination of π; however, as in the first example of this chapter, the rate of convergence is slow. It is very much in the spirit of inverting a probabilistic result to get a stochastic computation. We would call it an *analog* computation nowadays [4].

Lord Kelvin [5] appears to have used random sampling to aid in evaluating some time integrals of the kinetic energy that appear in the kinetic theory of gases. His random sampling consisted of drawing numbered pieces of paper from a bowl. He worried about the bias introduced by insufficient mixing of the papers and by static electricity. Gossett (as ''Student'' [6]) used similar random sampling to assist in his discovery of the distribution of the correlation coefficient.

Many advances were being made in probability theory and the theory of random walks that would be used in the foundations of Monte Carlo theory. For example, Courant *et al.* [7] showed the equivalence of the behavior of certain random walks to solutions of certain partial differential equations. In the 1930s, Enrico Fermi made some numerical experiments that would now be called *Monte Carlo calculations*.[1)] In studying the behavior of the newly discovered neutron, he carried out sampling experiments about how a neutral particle might be expected to interact with condensed matter. These led to substantial physical insight and to the analytical theory of neutron diffusion and transport.

During the Second World War, the bringing together of such people as von Neumann, Fermi, Ulam, and Metropolis and the beginnings of modern digital computers gave a strong impetus to the advancement of Monte Carlo. In the late 1940s and early 1950s, there was a surge of interest. Papers appeared that described the new method and how it could be used to solve problems in statistical mechanics, radiation transport, economic modeling, and other fields [8–10]. Unfortunately, the computers of that time were not really adequate to carry out more than pilot studies in many areas. The later growth of computer power made

1) This information was communicated privately to MHK by Segre and Anderson.

it possible to carry through more and more ambitious calculations and to learn from failures.

At the same time, theoretical advances and putting into practice powerful error-reduction methods meant that applications advanced far faster than implied by sheer computing speed and memory size. The two most influential developments of that kind were the improvements in methods for the transport equation, especially reliable methods of ''importance sampling'' [11] and the invention of the algorithm of Metropolis *et al*. [12]. The resulting successes have borne out the optimistic expectations of the pioneers of the 1940s.

References

1 Ulam, S. (**1976**) *Adventures of a Mathematician*, Charles Scribner's & Sons, New York, pp. 196–97.

2 Comte de Buffon, G. (**1777**) Essai d'arithmétique morale. *Supplément à l'Histoire Naturelle*, **4**, Paris: de L'Imprimerie Royale.

3 Pierre-Simon de Laplace, M. (**1886**) Theorie analytique des probabilités, livre 2, *Oeuvres Compleétes de Laplace*, Vol. 7, Part 2, L'Acadeémie des Sciences, Paris, pp. 365–66.

4 Kendall, M.G. and Moran, P.A.P. (**1963**) *Geometrical Probability*, Hafner Publishing Company, New York. Monte Carlo applications of Buffon's problems are discussed on pp. 70–73.

5 Kelvin, L. (**1901**) Nineteenth century clouds over the dynamical theory of heat and light. *Philosophical Magazine, Series 6*, **2**, 1.

6 Student (**1908**) Probable error of a correlation coefficient. *Biometrika*, **6**, 302.

7 Courant, R., Friedrichs, K.O. and Lewy, H. (**1928**) On the partial difference equations of mathematical physics. *Mathematische Annalen*, **100**, 32.

8 Metropolis, N. and Ulam, S. (**1949**) The Monte Carlo method. *Journal of the American Statistical Association*, **44**, 335.

9 Donsker, M.C. and Kac, M. (**1950**) The Monte Carlo method and its applications, *Proceedings, Seminar on Scientific Computation*, November, 1949, International Business Machines Corporation, New York, pp. 74–81.

10 Householder, A.S., Forsythe, G.E. and Germond, H.H. (eds) (**1951**) *Monte Carlo Methods, National Bureau of Standards Applied Mathematics Series*, Vol. 12, p. 6.

11 Kahn, H. (**1950**) Modifications of the Monte Carlo method, *Proceedings, Seminar on Scientific Computation*, November, 1949, International Business Machines Corporation, New York, pp. 20–27.

12 Metropolis, N., Rosenbluth, A.W., Rosenbluth, M.N. *et al*. (**1953**) Equations of state calculations by fast computing machines. *The Journal of Chemical Physics*, **21**, 1087.

2
A Bit of Probability

2.1
Random Events

As explained in Chapter 1, a Monte Carlo calculation is a numerical stochastic process, that is, a sequence of random events. While we shall not discuss the philosophical question of what random events are [1, 2], we shall assume that they do exist and that it is possible and useful to develop a computer program to produce effective equivalents of natural random events.

We must distinguish between elementary and composite events. Elementary events are those that we cannot (or do not choose to) analyze into still simpler events. Normally the result (head or tail) of flipping a coin or the result (1–6) of rolling a die are thought of as elementary events. In the case of a die, however, we might interest ourselves only in whether the number was even or odd, in which case there are two outcomes. Composite events are those defined from a number of elementary events. Examples include flipping a coin twice (with four outcomes, head–head, head–tail, tail–head, tail–tail). It is sometimes useful to talk of this pair as a single ''event''.

As far as one knows, random events occur in nature [3]; for example, the physical outcome of the scattering of an electron by an atom cannot be predicted with certainty. It is difficult to be sure which natural random events are ''elementary,'' although we will simplify models of physical processes by treating some events as elementary, and on that basis build up composite events. The distinction between an elementary random event and others depends on one's state of knowledge and the depth of the analysis given to the problem. Thus, one important kind of event, ''compound elastic scattering'' of neutrons by nuclei, is usefully analyzed for theoretical purposes into a sequence of three elementary random events. A Monte Carlo calculation might or might not make that distinction, depending on its intent. On the other hand, ''simple elastic scattering'' is most likely an elementary event; that is, it is not possible to distinguish more basic stages.

Given an elementary event with a countable set of discrete random outcomes, $E_1, E_2, \ldots, E_n, \ldots$, there is associated with each possible outcome E_k a number called a *probability*, p_k, which can lie between 0 and 1,

$$0 \leq p_k \leq 1.$$

Monte Carlo Methods. Second Edition. M.H. Kalos and P.A. Whitlock

ISBN: 978-3-527-40760-6

If the kth outcome never occurs, $p_k = 0$; if it is sure to occur, $p_k = 1$. Conversely, if $p_k = 0$, we say that the event almost surely does not occur; and if $p_k = 1$, the event almost surely occurs. Another notation for the probability of event E_k is

$$P\{E_k\} = p_k.$$

The following are some simple properties of the probability of events:

1. $P\{E_i \text{ and/or } E_j\} \leq p_i + p_j$.
2. E_i and E_j are said to be *mutually exclusive events* if and only if the occurrence of E_i implies that E_j does not occur, $E_i \Rightarrow \overline{E}_j$ (not E_j), and vice versa. If E_i and E_j are mutually exclusive,

   $$P\{E_i \text{ and } E_j\} = 0,$$

   $$P\{E_i \text{ or } E_j\} = p_i + p_j.$$

3. A whole class of events can be mutually exclusive for all i and j. When the class is exhaustive, that is, all *possible* events have been enumerated,

   $$P\{\text{some } E_i\} = \sum_i p_i = 1.$$

   In the following, we consider a compound experiment consisting of just two elementary events. For clarity, we imagine the first to have outcomes $\{E_i\}$ with probability p_{1i} and the second to have outcomes $\{F_j\}$ and probabilities p_{2j}, respectively. Each of p_{1j} and p_{2j} obeys statements 1, 2, and 3 above. An outcome of such a composite event is a pair (E_i, F_j).
4. The probability of the specific outcome (E_i, F_j) is p_{ij}, called the *joint probability* for E_i and F_j.
5. $p_{ij} = p_{1i} \cdot p_{2j}$, if and only if events E_i and F_j are independent.
6. Suppose E_i and F_j are not independent; then the joint probability can be written as

   $$p_{ij} = \left(\sum_k p_{ik}\right)\left[\frac{p_{ij}}{\sum_k p_{ik}}\right]$$

   $$= p(i)\left[\frac{p_{ij}}{\sum_k p_{ik}}\right]. \tag{2.1}$$

   $p(i)$ defines a new number called the *marginal probability for event* E_i, that is, the probability that E_i does, in fact, occur, whatever the second event may be. Therefore,

   $$\sum_i p(i) = \sum_i \sum_k p_{ik} = 1 \text{ and } p(i) = p_{1i}.$$

The marginal distribution for the second event, F_j, can be similarly be written as $\sum_i p_{ij}$.

7. The second factor of Equation 2.1 is the conditional probability

$$p(j|i) \equiv \frac{p_{ij}}{\sum_k p_{ik}} \tag{2.2}$$

and is the probability for event F_j occurring, given that event E_i has occurred. The probability for *some* F_j should be 1, and indeed

$$\sum_j p(j|i) = \sum_j \frac{p_{ij}}{\sum_k p_{ik}} = \frac{\sum_j p_{ij}}{\sum_k p_{ik}} = 1 \text{ for every } i.$$

All joint probabilities can be factored into a marginal distribution and a conditional probability. This scheme can be generalized to treat the joint occurrence of three or more elementary events.

2.2 Random Variables

In many cases, the outcome of a random event can be mapped into a numerical value, but in some circumstances this is not possible (the probability of an event is always defined, but the assigning of a number to each outcome of a class of random events may not be useful). For example, when a photon interacts with an atom, the photon may be scattered or it may cause other changes to happen within the atom. There is no useful way to assign a numerical value to correspond to the alternative changes. In simulating a queue, an empty queue could be equated with length 0, but the meaning of the empty queue is really logical, not numerical. It implies that some other course of action must be taken. In general, with simulations on the computer, the outcome of a random choice is often a logical event; it may imply that a different branch of the program is to be pursued. In the following discussion, however, we shall assume that for every elementary outcome E_i, there is an associated real number x_i. A random selection, X, of one of the possible values $x_1, x_2, \ldots$ is called a *random variable*. The probability that the value x_i is chosen is given by $p_i = P\{X = x_i\}$.

The *expectation* of this random variable X, that is, the stochastic mean value, is defined as

$$E(X) \equiv \sum_i P\{X = x_i\} x_i = \sum_i p_i x_i = \mu. \tag{2.3}$$

μ is called the *expected or mean value*. It is common in physics to write this as $\langle X \rangle$, and we shall often use that notation.

Consider some real-valued function

$$g(x_i) = g_i,$$

where the x_i correspond to a countable set of elementary events with probabilities p_i. If X is a random variable, then $g(X)$ is also a random variable. The expectation of $g(X)$ is defined as

$$E(g(X)) = \langle g(X) \rangle = \sum_i p_i g(x_i). \tag{2.4}$$

This may be illustrated by analyzing the flipping of a coin, assigning 1 to heads, 0 to tails and using two different functions $g_1(X)$ and $g_2(X)$.

From the definition of the expected value of a function, we have the property that

$$\langle \text{constant} \rangle = \text{constant}$$

and that for any constants λ_1, λ_2 and two functions g_1, g_2,

$$\langle \lambda_1 g_1(X) + \lambda_2 g_2(X) \rangle = \lambda_1 \langle g_1(X) \rangle + \lambda_2 \langle g_2(X) \rangle. \tag{2.5}$$

In Table 2.1, g_1 is a linear function of X, so that

$$\langle g_1(X) \rangle = g_1(\langle X \rangle).$$

This is not true for the nonlinear function $g_2(X)$.

An important application of expected values is to the powers of X. The nth moment of X is defined as the expectation of the nth power of X,

$$\langle X^n \rangle \equiv \sum_i p_i x_i^n; \tag{2.6}$$

for example,

$$\langle X^2 \rangle = \sum_i p_i x_i^2.$$

The central moments of X are given by

$$\langle g_n \langle X \rangle \rangle \equiv \langle (X - \mu)^n \rangle = \sum_i p_i (x_i - \langle X \rangle)^n. \tag{2.7}$$

The second central moment has particular significance,

$$\begin{aligned} \langle (X - \mu \rangle^2 \rangle = \langle (X - \langle X \rangle)^2 \rangle &= \sum_i p_i (x_i - \mu)^2 \\ &= \sum_i p_i x_i^2 - \langle X \rangle^2 = \langle X^2 \rangle - \langle X \rangle^2, \end{aligned} \tag{2.8}$$

Table 2.1 Expected values of two functions, $g_1(X)$ and $g_2(X)$, where X can be either 0 or 1.

Event		p_i	x_i	$g_1(x_i) = 1 + 3x_i$	$g_2(x_i) = \frac{1+3x_i}{1+x_i}$
E_1	Heads	$\frac{1}{2}$	1	4	2
E_2	Tails	$\frac{1}{2}$	0	1	1
Expected values			$\langle X \rangle = \frac{1}{2}$	$\langle g_1(X) \rangle = \frac{5}{2}$	$\langle g_2(X) \rangle = \frac{3}{2}$

and is called the *variance of X* or var{x}. The square root of the variance is a measure of the dispersion of the random variable. It is referred to as the *standard deviation* and sometimes the *standard error*. The variance of a function of the random variable, $g(X)$, can be determined as

$$\begin{aligned}\text{var}\{g(X)\} &= \langle (g(X) - \langle g(X)\rangle)^2\rangle \\ &= \sum_i p_i g^2(x_i) - \left(\sum_i p_i g(x_i)\right)^2 \\ &= \langle g(X)^2\rangle - \langle g(X)\rangle^2.\end{aligned} \tag{2.9}$$

Consider two real-valued functions, $g_1(X)$ and $g_2(X)$. They are both random variables, but they are not in general independent. Two random variables are said to be independent if they derive from independent events. As we have seen in Equation 2.5, the expectation of a linear combination is the linear combination of the expectations. This result does not require that $g_1(x)$ and $g_2(x)$ be independent. The effect of statistical dependence will be seen in the variance of a linear combination of the two functions,

$$\begin{aligned}\text{var}\{\lambda_1 g_1(X) + \lambda_2 g_2(X)\} = \lambda_1^2 \text{var}\{g_1(X)\} + \lambda_2^2 \text{var}\{g_2(X)\} \\ +2[\lambda_1\lambda_2\langle g_1(X)g_2(X)\rangle - \lambda_1\lambda_2\langle g_1(X)\rangle\langle g_2(X)\rangle].\end{aligned} \tag{2.10}$$

Let X and Y be random variables; the expectation of the product is

$$\langle XY\rangle = \sum_{i,j} p_{ij} x_i y_j. \tag{2.11}$$

If X and Y are independent, $p_{ij} = p_{1i}.p_{2j}$ and

$$\langle XY\rangle = \sum_i p_{1i} x_i \sum_j p_{2j} y_j = \langle X\rangle\langle Y\rangle.$$

The expectation of the product is now the product of the expectations. Let $g_1(X) = X$ and $g_2(Y) = Y$ in Equation 2.11 then the bracketed quantity would vanish and

$$\text{var}\{\lambda_1 X + \lambda_2 Y\} = \lambda_1^2 \text{var}\{X\} + \lambda_2^2 \text{var}\{Y\}. \tag{2.12}$$

When X and Y are not necessarily independent, we introduce a new quantity, the covariance, which is a measure of the degree of independence of the two random variables X and Y:

$$\text{cov}\{X, Y\} = \langle XY\rangle - \langle X\rangle\langle Y\rangle. \tag{2.13}$$

The covariance equals 0 when X and Y are independent and

$$\text{cov}\{X, X\} = \text{var}\{X\}.$$

Note that zero covariance does not by itself imply independence of the random variables. The following simple example illustrates that even functional dependence can still yield a zero covariance. Let X be a random variable that may be -1, 0, or 1 with equal probabilities, and define $Y = X^2$. Obviously,

$$\langle X \rangle = 0,$$
$$\langle XY \rangle = \langle X^3 \rangle = 0,$$

so $\text{cov}\{XY\} = \langle XY \rangle - \langle X \rangle \langle Y \rangle = 0$.

The covariance can have either a positive or negative value. Another quantity derived from the covariance is the correlation coefficient,

$$\rho(X, Y) = \frac{\text{cov}\{X, Y\}}{[\text{var}\{X\}\text{var}\{Y\}]^{1/2}}, \tag{2.14}$$

so that

$$-1 \leq \rho(X, Y) \leq 1.$$

Since the covariance can be positive or negative, the variance of a linear combination of two dependent random variables can be greater or less than the variance if the variables were independent (cf. Equation 2.11). A Monte Carlo calculation can try to take advantage of negative correlation as a means of reducing the variance, as will be discussed in Chapter 4.

2.2.1 The Binomial Distribution

Consider two events E_0 and E_1 that are mutually exclusive and exhaustive:

$$P\{E_1\} = p, \quad x_1 = 1,$$
$$P\{E_0\} = 1 - p, \quad x_0 = 0. \tag{2.15}$$

Let X_i be the random variable that is the ith outcome of a series of N such events. The expectations of X_i and its square become

$$E(X_i) = p \times 1 + (1 - p) \times 0 = p,$$
$$E(X_i^2) = p,$$

and the variance is then

$$\text{var}\{X_i\} = p - p^2 = p(1 - p).$$

Each outcome is either 0 or 1, and we set X to be the sum of the N outcomes $\{X_i\}$,

$$X = \sum_{i=1}^{N} X_i.$$

The probability that $X = n$ is the probability that n of the X_i were 1 and $N - n$ were 0. That is,

$$P\{X = n\} = \binom{N}{n} p^n (1-p)^{N-n} \quad n = 0, 1, \ldots, N. \tag{2.16}$$

This is the *binomial distribution.* $\binom{N}{n} = \dfrac{N!}{(N-n)!n!}$ is the binomial coefficient, which counts the number of different ways in which the n E_1's and the $(N - n)$ E_0's may occur. The expected value of X is

$$\langle X \rangle = \sum_{n=0}^{N} n \binom{N}{n} p^n (1-p)^{N-n} = Np. \tag{2.17}$$

This may be verified by direct computation of the sum or by noting that the expected value of X is the sum of the expected value of all the X_i. The variance of X is easily determined; since the X_i are independent, the result in Equation 2.12 may be employed and

$$\langle (X - Np)^2 \rangle = \sum_{i=1}^{N} \mathrm{var}\{X_i\} = \sum_{i=1}^{N} p(1-p) = Np(1-p). \tag{2.18}$$

2.2.2
The Geometric Distribution

Suppose we carry out a certain experiment repeatedly and Independently, where there are only two outcomes: failure or success. If the outcome is a failure, the experiment will be repeated; otherwise, we stop the procedure. Let the random variable X of interest be the number of times we repeat the experiment until the first success. Let q be the probability of failure in one experiment and $p = 1 - q$ be the probability of success.

Then

$$P\{X = n\} = q^{n-1}p, \; n = 1, 2, \ldots.$$

The average number of experiments that will be carried out is

$$\langle X \rangle = \sum_{n=1}^{\infty} nq^{n-1}p = \frac{p}{(1-q)^2} = \frac{1}{p}.$$

This is obtained from the identity

$$\sum_{n=1}^{\infty} nx^{n-1} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\sum_{n=0}^{\infty} x^n\right) = \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{1-x}\right) = \frac{1}{(1-x)^2}.$$

The above identity can also be used to prove Equation 2.17 by taking the Nth derivative of the sum.

The variance of X can be calculated as

$$\begin{aligned}\mathrm{var}\{X\} &= \langle X^2\rangle - \langle X\rangle^2 \\ &= \left(\frac{2}{p^2} - \frac{1}{p}\right) - \frac{1}{p^2} \\ &= \frac{1}{p^2} - \frac{1}{p}.\end{aligned}$$

As an example, in particle transport problems, the number of collisions one particle makes follows this distribution if the medium is infinite, homogeneous, and if the relative probability of different outcomes is constant.

2.2.3 The Poisson Distribution

A random variable X is said to follow a Poisson distribution when

$$P\{X = n\} = \frac{\lambda^n}{n!}\,\mathrm{e}^{-\lambda},\ n = 0, 1, \ldots,$$

where λ is a parameter of the distribution. It is easy to show that

$$\langle X\rangle = \lambda,$$

$$\mathrm{var}\{X\} = \lambda.$$

This distribution is fundamental in the theory of probability and stochastic processes. It is of great use in applications such as research into queuing service systems and similar discrete event problems.

2.3 Continuous Random Variables

In the previous sections, we have assumed that the random events belonged to a discrete, countable set. Probabilities can be associated with continuous variables as well, giving rise to distribution functions. Such distributions are present both in nature and in artificial stochastic processes. As an example, consider the scattering of a photon by an atom. The angle at which the photon is scattered has values that are continuous between 0° and 180° with some angular intervals occurring more often than others.

Given that x is a real number,

$$-\infty < x < \infty,$$

a distribution function (or *cumulative* distribution function) may be defined as

$$F(x) \equiv P\{\text{a random selection of } X \text{ gives a value less than } x\} = P\{X \leq x\}. \quad (2.19)$$

Suppose $x_1 < x_2$. Then $x_1 < X \leq x_2$, and $X \leq x_1$ are mutually exclusive and exhaustive for events in which $X \leq x_2$. Thus

$$P\{x_1 < X \leq x_2\} + P\{X \leq x_1\} = P\{X \leq x_2\} \tag{2.20}$$

and

$$1 \geq P\{x_1 < X \leq x_2\} = P\{X \leq x_2\} - P\{X \leq x_1\} \geq 0. \tag{2.21}$$

Therefore, $F(x)$ is a nondecreasing function of its argument. We conclude that $F(-\infty) = 0$ and $F(\infty) = 1$. Furthermore, the difference $P\{X \leq x_2\} - P\{X \leq x_1\}$ may be written as $F(x_2) - F(x_1)$.

The distribution function may have intervals on which it is differentiable; in these intervals, the probability distribution function (pdf) may be defined as

$$f(x) \equiv \frac{\mathrm{d}F(x)}{\mathrm{d}x} \geq 0. \tag{2.22}$$

If $F(x)$ is not continuous, discrete values of the distribution function are singled out at the discontinuities. For example, imagine that $F(x)$ is piecewise constant everywhere except at a countable number of places (Figure 2.1); the distribution now describes a discrete set of random variables. Formally, we may use the Dirac *delta function* to write

$$f(x) = \sum_i \delta(x - x_i) \times p_i, \tag{2.23}$$

where p_i is the jump of the distribution function at x_i. This emphasizes the fact that $f(x)$ need not be bounded.

Consider the distribution function shown in Figure 2.2. $F(x) = 0$ for all $x \leq 0$, so no X will be chosen there and the pdf $= 0$. In region II, $0 < x < 1$ and $F(x) = x$; the probability of selecting an X in the interval $0 \leq x_1 < X \leq x_2 \leq 1$ is $x_2 - x_1$ (see Equation 2.21). In this range, the pdf $= 1$, so that selecting a particular X is as likely as any other on $(0, 1)$. For $x > 1$, $F(x) = 1$, and the probability of choosing an X in this region is 0.

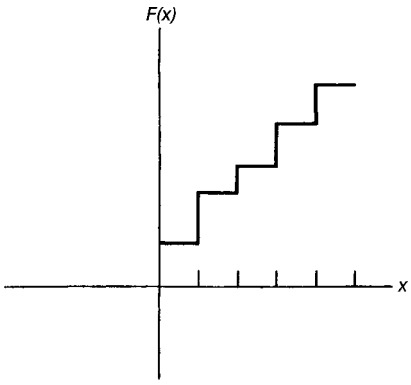


Figure 2.1 A piecewise-constant function.

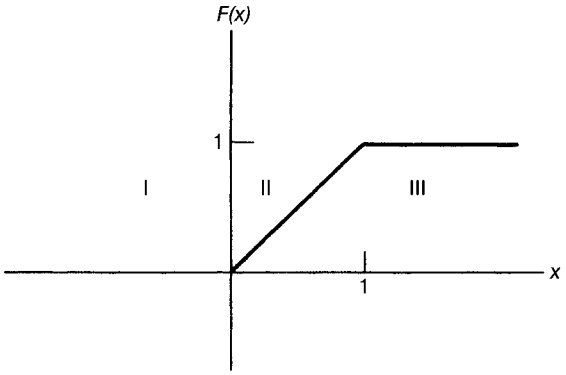


Figure 2.2 A discontinuous distribution function.

A slightly different example is the discontinuous distribution function in which $F(x)$ has a step discontinuity from 0 to $\frac{1}{2}$ at $x = 0$ shown in Figure 2.3. No matter how small an interval is chosen containing $x = 0$, the probability of choosing an X in this interval is greater than or equal to $\frac{1}{2}$, so there is a finite probability, $\frac{1}{2}$, for finding X exactly 0. For any other value of x, the pdf is continuous. We have a combination of a discrete and a continuous pdf. Such combinations occur in nature, for example, when an atom can undergo a radiative transition to either a continuum or a discrete level. The light spectrum, which may be considered as a pdf, will be a mixture of a continuous and a discrete part.

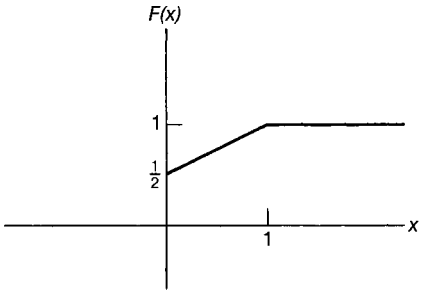


Figure 2.3 Discontinuous distribution function with a step discontinuity.

2.4 Expectations of Continuous Random Variables

Let $f(x)$ be the pdf of a continuous random variable x. It has the normalization property

$$\int_{-\infty}^{\infty} f(x)\,dx = F(\infty) = 1.$$

The mean value of x is defined as

$$E(X) \equiv \int_{-\infty}^{\infty} x \, \mathrm{d}F(x)$$
$$= \int_{-\infty}^{\infty} xf(x) \, \mathrm{d}x, \tag{2.24}$$

The expected value of any function of the random variable is defined[1)] as

$$E(g(X)) \equiv \int_{-\infty}^{\infty} g(x)f(x) \, \mathrm{d}x,$$

and, in particular,

$$E(X^2) = \int_{-\infty}^{\infty} x^2 f(x) \, \mathrm{d}x. \tag{2.25}$$

From Equations 2.24 and 2.25, the variance of X may be defined as in the discrete case

$$\mathrm{var}\{X\} = E((X - E(X))^2) = E(X^2) - [E(X)]^2 = \langle X^2 \rangle - \langle X \rangle^2. \tag{2.26}$$

The variance of a function of X becomes

$$\mathrm{var}\{g(X)\} = E(g^2(X)) - [E(g(X))]^2. \tag{2.27}$$

The variance has the following properties:

1. For a random variable C, which is constant (i.e. the random variable equals C with probability 1),

   $$\mathrm{var}\{C\} = 0.$$

2. For a constant C and random variable X,

   $$\mathrm{var}\{CX\} = C^2 \mathrm{var}\{X\}.$$

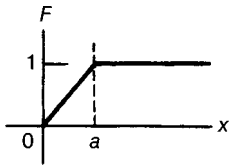
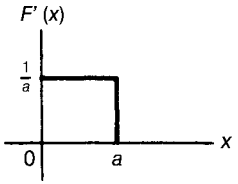
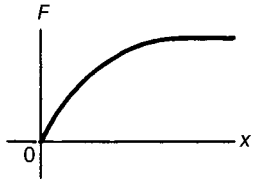
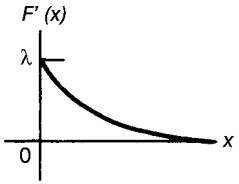
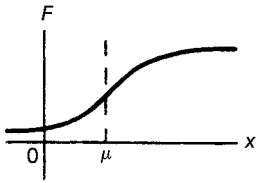
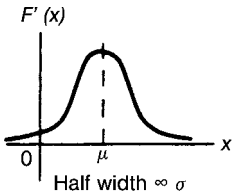
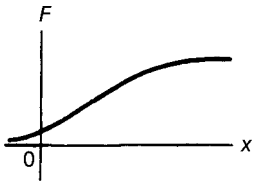
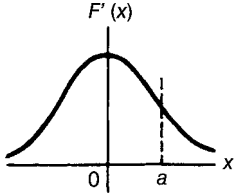
3. For independent random variables X and Y,

   $$\mathrm{var}\{X + Y\} = \mathrm{var}\{X\} + \mathrm{var}\{Y\}.$$

In Table 2.2, $F(x), f(x) = F'(x)$, the mean and variance are given for a few representative and interesting distributions. In particular, the mean value of a random variable drawn from a normal distribution centered around μ is μ. This result is easily proved by considering the following integral:

1) Since $g(X)$ is a random variable, it has its own pdf; we will show below how to compute it. Given this distribution, the expectation of $g(X)$ could be alternatively defined in the same way as in Equation 2.24. It can be proved that both the definitions will be the same [4].

Table 2.2 Continuous probability distribution function.

Distribution function	$F(x)$		$F'(x)$		$\langle x \rangle$	var(x)
Uniform	$0,\ x < 0$ $x,\ 0 \le x \le a$ $1,\ x > a$		$0, x < 0, x > a$ $\frac{1}{a}, 0 < x < a$		$\frac{1}{2}a$	$\frac{1}{12}a$
Exponential	$0, \quad x < 0$ $1 - \exp(-\lambda x),\ x \ge 0$		$0, \quad x < 0$ $1 - \exp(-\lambda x),\ x \ge 0$		$\frac{1}{\lambda}$	$\frac{1}{\lambda^2}$
Normal $\phi(x\|\mu\sigma)$ μ = mean σ^2 = variance	$\frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{x}$ $\times \exp\left\|\frac{-(t-\mu)^2}{2\sigma^2}\right\| dt$		$\frac{1}{\sigma\sqrt{2\pi}} \exp\left\|-\frac{(x-\mu)^2}{2\sigma^2}\right\| dt$		μ	σ^2
Cauchy (Lorentz)	$\frac{1}{2} + \frac{1}{\pi}\tan^{-1}\left(\frac{x}{a}\right)$		$\frac{a}{a^2 + x^2}$		?	∞

$$\frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty}(x-\mu)\exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]\,dx,$$

which equals 0 since the integrand changes sign on reflection of x about μ. The integral may be rewritten as

$$\frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty}x\exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]dx=\mu\frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]\,dx.$$

The integral on the right-hand side is just the integral of the pdf and it equals 1. The mean value of X is seen to be μ. The variance is σ^2.

A less well-behaved example is provided by the Cauchy or Lorentz function. The mean value of a random variable sampled from a Cauchy distribution is

$$\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{ax}{a^2+x^2}\,dx.$$

To evaluate this improper integral using elementary calculus, the infinite endpoints of integration are replaced by finite quantities b and b', and the behavior of the integrand as b and b' approach infinity is considered. The integrand clearly diverges unless $b=b'$, and then the mean value is 0. This suggests that the mean value of a series of random variables may be undefined unless the variables are chosen in some special way. The variance of a random variable sampled from a Cauchy distribution is infinity since the integral

$$\langle X^2\rangle=\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{ax^2}{a^2+x^2}\,dx$$

diverges no matter how it is evaluated. In spite of the infinite variance, the Cauchy distribution can be sampled and used as needed.

Note that for each distribution there is a length scale, called variously a, λ^{-1}, or σ. As the scale becomes small, the normalization of the pdf grows large, inversely as the length scale, so as to ensure $\int f(x)\,dx=1$. For those distributions with a standard deviation σ, the width is proportional to σ. In the Cauchy distribution, a is a measure of the width.

2.5
Bivariate Continuous Random Distributions

A joint probability may be defined for continuous distributions,

$$F(x,y)\equiv P\{X\le x, Y\le y\};\tag{2.28}$$

$F(x,y)$ is termed a *bivariate distribution* function. The associated bivariate probability distribution function is

$$f(x,y)\equiv\frac{\partial^2F(x,y)}{\partial x\partial y}\tag{2.29}$$

and the expected value of any function of random variables X, Y is

$$E(g(X, Y)) = \langle g(X, Y)\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x, y)g(x, y)\,\mathrm{d}x\,\mathrm{d}y. \tag{2.30}$$

The covariance and correlation coefficient, $\mathrm{cov}\{X, Y\}$ and $\rho(X, Y)$ for continuous random variables are defined as in the discrete case, replacing sums by integrals.

If X and Y are correlated, it is useful to write the joint pdf as

$$f(x, y) = \frac{f(x, y)}{\int_{-\infty}^{\infty} f(x, y)\,\mathrm{d}y}\int_{-\infty}^{\infty} f(x, y)\,\mathrm{d}y. \tag{2.31}$$

We have

$$P\{X \le x\} = \int_{-\infty}^{x}\int_{-\infty}^{\infty} f(t, y)\,\mathrm{d}y\,\mathrm{d}t = \int_{-\infty}^{x} m(t)\,\mathrm{d}t,$$

where

$$m(x) \equiv \int_{-\infty}^{\infty} f(x, y)\,\mathrm{d}y, \tag{2.32}$$

is called the *marginal probability distribution function* for x. The first factor in Equation 2.31 is the conditional probability; that is, given an X, a Y may be chosen from

$$f(y|x) = \frac{f(x, y)}{\int_{-\infty}^{\infty} f(x, y)\,\mathrm{d}y} = \frac{f(x, y)}{m(x)}. \tag{2.33}$$

That is, when the marginal and conditional functions can be determined, sampling a bivariate distribution requires simply sampling two univariate distributions.

The relationship in Equation 2.31 is easily generalized to handle more than two correlated random variables, and sampling the multivariate distribution will then involve sampling the sequence of univariate distributions so defined. What happens to the marginal pdf and the conditional probability when X and Y are independent (i.e. $f(x, y) = f_1(x)f_2(y)$) is left for the reader.

The expectation of the conditional probability, called the *conditional expectation* of Y, for fixed X is

$$\begin{aligned} E(Y|X) &\equiv \int_{-\infty}^{\infty} y f(y|x)\,\mathrm{d}y = \frac{\int_{-\infty}^{\infty} y f(x, y)\,\mathrm{d}y}{\int_{-\infty}^{\infty} f(x, y)\,\mathrm{d}y} \\ &= \frac{\int_{-\infty}^{\infty} y f(x, y)\,\mathrm{d}y}{m(x)}. \end{aligned}$$

The conditional expectation $E(Y|X)$ is a function of the random variable X and is itself a random variable. The expectation of $E(Y|X)$ is

$$E(E(Y|X)) = \int_{-\infty}^{\infty} E(Y|X)\, m(x)\,\mathrm{d}x.$$

Upon substituting in the definition for $E(Y|X)$

$$\begin{aligned} E(E(Y|X)) &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} y f(x, y)\,\mathrm{d}y\,\mathrm{d}x \\ &= E(Y). \end{aligned}$$

A more general result for a function g(X,Y) is

$$E(E(g(X, Y)|X)) = E(g(X, Y)).$$

This result is very useful in the discussion of the "method of expected values" discussed in Section 4.2.

2.6
Sums of Random Variables: Monte Carlo Quadrature

Suppose that the random variables $X_1, X_2, \ldots, X_i, \ldots$ are all drawn at random, but not necessarily independently, from the probability distribution function $f(x)$. Let g_i be a (possibly) different function of X_i and λ_i a real number. Define the function G by

$$G \equiv \sum_{i=1}^{N} \lambda_i g_i(X_i), \tag{2.34}$$

The expected value of G is

$$\begin{aligned} E(G) = \langle G \rangle &= E\left(\sum_{i=1}^{N} \lambda_i g_i(X_i)\right) \\ &= \sum_{i=1}^{N} \lambda_i \langle g_i(X) \rangle, \end{aligned} \tag{2.35}$$

since the expectation is a linear operation. If all the X_i are independent, then the variance of G,

$$\mathrm{var}\{G\} = \langle G^2 \rangle - \langle G \rangle^2,$$

becomes

$$\mathrm{var}\{G\} = \sum_{i=1}^{N} \lambda_i^2 \mathrm{var}\{g_i(X)\}. \tag{2.36}$$

Let $\lambda_i = \frac{1}{N}$ and all the $g_i(x)$ be identical and equal to $g(x)$; then the expected value of G becomes

$$\begin{aligned} E(G) &= E\left(\frac{1}{N}\sum_{i=1}^{N} g(X_i)\right) \\ &= \frac{1}{N}\sum_{i=1}^{N} \langle g(X) \rangle = \langle g(X) \rangle. \end{aligned} \tag{2.37}$$

The function G, which is the arithmetic average of the $g(x)$, has the same mean as $g(x)$. G is said to be an *estimator* of $\langle g(X) \rangle$. More generally an expression

G is an estimator of a quantity, such as $\int g(x)f(x)\,dx)$, if its mean $\langle G\rangle$ is a useful approximation of that quantity. Here, "useful" is intended to cover a broad range of meanings, and is best understood in the context of specific computations. We will discuss this more fully below in connection with some applications.

The variance of G in Equation 2.36 becomes

$$\begin{aligned}\mathrm{var}\{G\} &= \mathrm{var}\left\{\frac{1}{N}\sum_{i=1}^{N} g(X_i)\right\} = \sum \frac{1}{N^2}\mathrm{var}\{g(X)\} \\ &= \frac{1}{N}\mathrm{var}\{g(X)\}. \end{aligned} \tag{2.38}$$

That is, as N, the number of samples of X, increases, the variance of the mean value of G decreases as $\frac{1}{N}$. This result leads to the central idea of Monte Carlo evaluation of integrals; that is, an integral may be estimated by a sum

$$\langle g(X)\rangle = \int_{-\infty}^{\infty} g(x)f(x)\,dx = E\left(\frac{1}{N}\sum_{i=1}^{N} g(X_i)\right). \tag{2.39}$$

To use the relation given in Equation 2.39, select a series of random variables, X_i, from $f(x)$; evaluate $g(x)$ for each X_i. The arithmetic mean of all the values of $g(X_i)$ is an estimate of the integral, and the variance of this estimate decreases as the number of terms increases.

2.7
Distribution of the Mean of a Random Variable: A Fundamental Theorem

In the discussion that follows on estimating integrals, it is assumed that the variance of the random variable always exists. If the variance does not exist, the mean value will converge, although more slowly. Alternatively, it will usually be possible to recast the sampling so that the variance does exist. A general method for doing this, along with several examples, will be given in Chapter 3.

The most general result of the kind we need is the "law of large numbers" of probability theory. Suppose the random variables $X_1, X_2, \ldots, X_N$ are independent and all drawn from the same distribution. These are called *independent, identically distributed* (or *i.i.d.*) random variables. Then the expectation of each X is μ. As $N \to \infty$, the average value of the $\{X_i\}$,

$$\overline{X}_N = \frac{1}{N}\sum_{i=1}^{N} X_i,$$

converges to μ almost surely:

$$P\{\lim_{N\to\infty} \overline{X}_N = \mu\} = 1.$$

There are stronger or weaker statements that can be made, but we shall not pursue them [5].

The implication of the law of large numbers is that the mean of N sampled random variables converges (in probability) to its expected value. To estimate the speed of convergence, we need stronger assumptions. The most important way of strengthening the hypothesis is to assume that the variance exists, which we do in the following.

Assume that an estimator G, its mean $\langle G \rangle$, and variance var$\{G\}$ all exist. Then the Chebychev inequality is

$$P\left\{|G - \langle G\rangle| \geq \left[\frac{\text{var}\{G\}}{\delta}\right]^{\frac{1}{2}}\right\} \leq \delta, \tag{2.40}$$

where δ is any positive number. This inequality could be called the *first fundamental theorem of Monte Carlo* for it gives an estimation of the chances of generating a large deviation in a Monte Carlo calculation. For definiteness, let $\delta = \frac{1}{100}$. Then the inequality becomes

$$P\{(G - \langle G\rangle)^2 \geq 100\ \text{var}\{G\}\} \leq \frac{1}{100}$$

or, using Equation 2.38 when var$\{G\} = \left(\frac{1}{N}\right)$ var$\{g\}$,

$$P\left\{(G - \langle G\rangle)^2 \geq \frac{100}{N}\ \text{var}\{g\}\right\} \leq \frac{1}{100}.$$

Since by making N big enough, the variance of G becomes as small as one likes, the probability of getting a large deviation relative to δ between the estimate of the integral and the actual value becomes very small. For large sample size (large N), the range of values of G that will be observed with some fixed probability will be contained in a region of decreasing size near $\langle g \rangle$. This is the heart of the Monte Carlo method for evaluating integrals.

A much stronger statement than the Chebychev inequality about the range of values of G that can be observed is given by the central limit theorem of probability. For any fixed value of N, there is a pdf that describes the values of G that occur in the course of a Monte Carlo calculation.[2)] As $N \to \infty$, however, the central limit theorem shows that there is a specific limit distribution for the observed values of G, namely, the normal distribution (see Section 2.4). Set

$$G_N = \frac{1}{N}\sum_{i=1}^{N} g(X_i)$$

and

$$\begin{aligned} t_N &= (G_N - \langle g(X)\rangle)/[\text{var}\{G_N\}]^{\frac{1}{2}} \\ &= \frac{\sqrt{N}(G_N - \langle g(X)\rangle)}{[\text{var}\{g(X)\}]^{\frac{1}{2}}}; \end{aligned}$$

2) For fixed N, if G was calculated M times, each time with a different sequence of i.i.d. random variables, the set $\{G_j\}$, $j = 1, \ldots, M$ has a specific distribution function.

then

$$\lim_{N\to\infty} P\{a < t_N < b\} = \int_a^b \frac{\exp[-t^2/2]\,dt}{\sqrt{2\pi}}. \tag{2.41}$$

Let $\sigma^2 = \text{var}\{g\}$. Equation 2.41 can be rewritten so as to specify a probability distribution function for values of G_N:

$$f(G_N) = \frac{1}{\sqrt{2\pi(\sigma^2/N)}} \exp\left[\frac{N(G_N - \langle g\rangle)2}{2\sigma^2}\right].$$

As $N \to \infty$, the observed G_N turns up in ever narrower intervals near $\langle g\rangle$ and one can predict the probability of deviations measured in units of σ. That is, the observed G_N is within one *standard error* (i.e. $\sigma/\sqrt{N}$) of $\langle g\rangle$ 68.3% of the time, within two standard errors of $\langle g\rangle$ 95.4% of the time, and within three standard errors 99.7% of the time.

The central limit theorem is very powerful in that it gives a specific distribution for the values of G_N, but it applies only asymptotically. How large N must be before the central limit theorem applies depends on the problem. If for a particular problem the third central moment μ_3 (Equation 2.7) of g exists, then the central limit theorem will be substantially satisfied when

$$|\mu_3| << \sigma^3\sqrt{N}.$$

Then confidence limits derived from the normal distribution can be applied to the results of a Monte Carlo calculation.

It is possible to calculate confidence limits exactly for the average of N variables drawn from certain distributions, such as the exponential distribution, $\exp(-x)$, $0 \leq x < \infty$. For this distribution, $\sigma = 1$; $\mu_3 = 2$. Table 2.3 gives the chance that the mean $\overline{x}$ of N random variables drawn from this distribution differs from μ by σ or 2σ on either side. Since the exponential distribution is skewed – there are no negative values of x – there are more large values of the average than predicted from the normal distribution. The last column shows that the total probability for deviations more than two standard deviations, large and small, converges quickly to

Table 2.3 Confidence limits for the exponential distribution as N increases.

N	$\sqrt{N}$	$\overline{x} < \mu - 2\sigma$	$\overline{x} < \mu - \sigma$	$\overline{x} > \mu + \sigma$	$\overline{x} > \mu + 2\sigma$	$\lvert\overline{x} - \mu\rvert > 2\sigma$
5	2.24	0.00022	0.1468	0.1525	0.04098	0.04120
10	3.16	0.00463	0.1534	0.1554	0.03685	0.04148
20	4.47	0.00977	0.1563	0.1569	0.03335	0.04312
50	7.07	0.01466	0.1578	0.1579	0.02981	0.04447
100	10	0.01711	0.1582	0.1583	0.02786	0.04497
200	14.14	0.01881	0.1584	0.1585	0.02643	0.04524
500	22.36	0.02028	0.1586	0.1586	0.02511	0.04539
Normal		0.02275	0.1587	0.1587	0.02275	0.04550

that given by the normal distribution. Whether this distinction matters will depend upon the application.

Without the central limit theorem, there is in general only the much weaker upper bound of the Chebychev inequality to suggest how much the observed G_N deviates from the actual mean. Of course, in specific cases, studies can be made of the distribution of the estimator. Much Monte Carlo is done assuming that the theorem has been satisfied no matter what the sample size; reported errors must be considered optimistic in such cases.

When the variance is infinite, it is sometimes possible to find a limit distribution for G that will lead to a central limit theorem for that particular problem. The limit distribution will in general not be normal. The Cauchy distribution yields an elementary example, as will be seen later.

The variance used in the discussion given above may itself be estimated using independent values of $g(x_n)$ in the following way:

$$\left\langle \frac{1}{N}\sum_{i=1}^{N} g^2(X_i) - \left[\frac{1}{N}\sum_{i=1}^{N} g(X_i)\right]^2 \right\rangle$$
$$= \langle g^2\rangle - \frac{1}{N^2}\left\langle \sum_{i=1}^{N} g(X_i)^2 + \sum_{i,i\neq j}^{N}\sum_{j=1}^{N} g(X_i)g(X_j)\right\rangle. \tag{2.42}$$

Using the independence of $g(X_i)$ and $g(X_j)$ in evaluating $\langle g(X_i)g(X_j)\rangle$, we find the right-hand side equal to

$$\left(1-\frac{1}{N}\right)\langle g^2\rangle - \frac{N(N-1)}{N^2}\langle g\rangle^2 = \frac{N-1}{N}\,\mathrm{var}\{g\}.$$

Thus an estimator for σ^2 is

$$\sigma^2 \approx \frac{N}{N-1}\left\{\frac{1}{N}\sum_{i=1}^{N} g^2(X_i) - \left(\frac{1}{N}\sum_{i=1}^{N} g(X_i)\right)^2\right\}. \tag{2.43}$$

An estimator of the variance of the estimated mean is given by

$$\mathrm{var}\{G_N\} \approx \frac{1}{N-1}\left\{\frac{1}{N}\sum_{i=1}^{N} g^2(X_i) - \left(\frac{1}{N}\sum_{i=1}^{N} g(X_i)\right)^2\right\}. \tag{2.44}$$

2.8
Distribution of Sums of Independent Random Variables

Let X be chosen from $f_1(x)$ and Y independently chosen from $f_2(y)$. If the sum $Z = X + Y$ is formed, what is the probability distribution function for Z? The distribution function is defined as

$$F_3(z) = P\{Z \le z\} = P\{X + Y \le z\}.$$

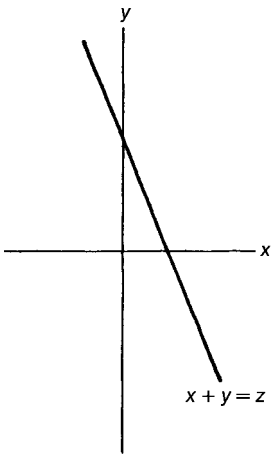


Figure 2.4 The sum of two random variables.

Since X and Y are independent, their joint probability distribution function is

$$f(x, y) = f_1(x) f_2(y).$$

The variables x and y can be considered to form a point in the xy plane (Figure 2.4). What fraction of the time does the point (x, y) lie below the line $X + Y = Z$? The (cumulative) distribution function is

$$\begin{aligned} F_3(z) &= \int_{x+y\le z} \int f_1(x) f_2(y)\, \mathrm{d}x\, \mathrm{d}y \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{z-x} f_2(y) f_1(x)\, \mathrm{d}y\, \mathrm{d}x. \end{aligned}$$

The cumulative distribution function of y is

$$F_2(y) = \int_{-\infty}^{y} f_2(u)\, \mathrm{d}u,$$

so

$$F_3(z) = \int_{-\infty}^{\infty} F_2(z - x) f_1(x)\, \mathrm{d}x. \tag{2.45}$$

Differentiating with respect to z, one obtains for the pdf of z

$$f_3(z) = \int_{-\infty}^{\infty} f_2(z - x) f_1(x)\, \mathrm{d}x.$$

This is a convolution and Fourier transforms can be used to evaluate it. Let

$$\begin{aligned} c_1(t) &= \int_{-\infty}^{\infty} \mathrm{e}^{ixt} f_1(x)\, \mathrm{d}x \\ &= E(\mathrm{e}^{iXt}). \end{aligned} \tag{2.46}$$

In probability theory, $c_1(t)$ is labeled the characteristic function of X. The characteristic function of the sum $(X + Y)$ is

$$\begin{aligned} c_3(t) &= E(\exp[i(X+Y)t]) \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp[i(x+y)t]\, f_1(x)\, f_2(y)\, \mathrm{d}x\, \mathrm{d}y \\ &= c_1(t)c_2(t), \end{aligned} \tag{2.47}$$

or the characteristic function of a sum is the product of the characteristic functions of the terms of the sum.[3)] Clearly, induction gives the same result for a sum of n variables. The characteristic function may be inverted (by a Fourier transform) to give the pdf to which it corresponds. If n identical functions constitute the sum, this result can be used to prove the central limit theorem.

When $F(x)$ is the normal distribution (Table 2.2), $\phi(x|0,1)$, the characteristic function is $\exp[-t^2/2]$. If a normal distribution is sampled n times, the sum is also distributed normally. The characteristic function is then $[c(t)]^n = \exp[-nt^2/2]$, which when inverted gives the normal distribution $\phi(x|0, n^{1/2})$. A similar conclusion follows for the Cauchy distribution; the characteristic function is $\exp[-|t|]$, and after n samples, the characteristic function of the sum is $[c(t)]^n = \exp[-n|t|]$. The distribution of the sum of n Cauchy variables has a Cauchy distribution and the ''width'' of this Cauchy distribution increases as n. As a final example, consider the exponential distribution $\lambda \exp[-\lambda t]$; its characteristic function is

$$c(t) = \frac{1}{1 - \frac{it}{\lambda}}.$$

Therefore, a sum of exponential random variables will not be distributed exponentially.

Note that the width of the distribution of the sum of n random variables increases with n. This is not contradictory with the earlier result on the mean of n random variables. It is not difficult to show – we shall prove it later – that if the characteristic distribution for x is $c(t)$, then the characteristic function x/n is $c(t/n)$. From this it follows that, if n variables are drawn from the normal distribution $\phi(x|0,1)$, then the mean has characteristic function $\exp[-(n/2)(t/n)^2] = \exp[-t^2/2n]$. This may be inverted to give the distribution function $\phi(x|0, n^{-\frac{1}{2}})$ for the mean. The latter shrinks with n as predicted by the central limit theorem. Indeed, we see that here the limiting behavior holds exactly for any n.

In the same way, the characteristic function for the mean of n Cauchy variables is $\exp[-n|t|/n] = \exp[-|t|]$. Thus the distribution of the mean is the same as for a single variable. Again the limit distribution for the mean is exact for any n, but now the distribution does not change its width. This does not, of course, satisfy the central limit theorem because the Cauchy distribution does not satisfy the requirement of a finite variance.

3) Note that if the two random variables are not independent, this statement is generally not true.

2.9 Monte Carlo Integration

We may summarize the important results of this chapter as follows. If $X_1, X_2, \ldots, X_n$ are i.i.d. random variables with probability distribution function $f(x)$ (x does not necessarily have to be in $\mathcal{R}^1$, i.e. be on the real line), then for a function g(x), an estimator is

$$G_N = \frac{1}{N}\sum_{i=1}^{N} g(X_i),$$

$$\langle G_N \rangle = \int_{-\infty}^{\infty} f(x)g(x)\,\mathrm{d}x,$$

and

$$\mathrm{var}\{G_N\} = \frac{1}{N}\mathrm{var}\{g\}.$$

As $N \to \infty$ and if the variance exists, the distribution of possible values of G_N narrows about the mean as $N^{-\frac{1}{2}}$; or the probability of finding a G_N some fixed distance away from $\langle G_N \rangle$ becomes smaller.

In the development of the Monte Carlo method so far, it has been assumed that the random variables are drawn from a continuous distribution function and that they are used to approximate an integral. Similar procedures can be employed to perform sums by Monte Carlo. It becomes advantageous to use Monte Carlo methods in the discrete case when many indices are involved. Consider the sum $\sum_i p_i g(X_i)$, where p_i is a discrete probability distribution. If random variables $X_1, \ldots, X_M$ are sampled from p_i and the quantity

$$G = \frac{1}{M}\sum_{i=1}^{M} g(X_i)$$

formed, the expected value of G is an estimator for the sum

$$\langle G \rangle = \sum p_i g(X_i).$$

Monte Carlo evaluation of a sum might be used to determine the probability of winning at solitaire; the probability is a finite sum, but contains a large number of terms. A sum over the permutations of L objects becomes cumbersome when L is large, but a Monte Carlo calculation can be performed efficiently.

The basic random variable used in Monte Carlo has been set by historical convention to be distributed uniformly between 0 and 1.

$$f_u(x) = 1, \quad 0 \le x \le 1.$$

The use of this random variable in integration is demonstrated in the following example:

$$\int_0^1 \sqrt{1-x^2}\,\mathrm{d}x = \frac{\pi}{4}. \tag{2.48}$$

It can be rewritten as

$$\int_0^1 f_u(x)\sqrt{1-x^2}\,\mathrm{d}x = \frac{\pi}{4},$$

The integral is now in a form in which we can apply the method described above for evaluating integrals. A uniform random variable ξ_i is sampled from $f_u(x)$, $g(\xi_i) = \sqrt{1-\xi_i^2}$ is calculated and this process is repeated N times to form

$$G_1 = \frac{1}{N}\sum g(\xi_i) = \frac{1}{N}\sum (1-\xi_i^2)^{\frac{1}{2}}. \tag{2.49}$$

The algorithm for calculating G_1 can be easily programmed. In the pseudocode that follows we shall use rand(u) as a generic name for a utility that produces good pseudorandom numbers uniform on $(0, 1)$ and assume that succeeding values returned by rand(u) are independent.

```
Initialize sum = 0
Repeat N times, i = 1, . . . , N
    sum = sum + sqrt(1.0 − rand(u)^2)
EndRepeat
mean = sum/N
```

However, the evaluation of the integral in Equation 2.48 by Monte Carlo can be approached in an entirely different manner.

Consider the unit square in the xy plane and the circle with unit radius (Figure 2.5). Integrating over the unit square but counting only those pairs of x and y that lie within the quarter circle yields the area of the quarter circle. That is

$$\int_0^1 \int_0^1 f(x,y)g(x,y)\,\mathrm{d}x\,\mathrm{d}y = \frac{\pi}{4},$$

where

$$f(x,y) = \begin{cases} 1 & (x,y) \text{ in } (0,1)\otimes(0,1) \text{ (i.e. inside the unit square)} \\ 0 & \text{otherwise} \end{cases}$$

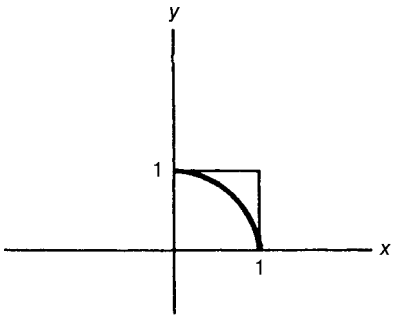


Figure 2.5 Unit square with inscribed quarter circle.

and

$$g(x,y) = \begin{cases} 1, & x^2 + y^2 \leq 1 \\ 0, & x^2 + y^2 > 1. \end{cases}$$

Since x and y are independent,

$$f(x,y) = f_u(x)\, f_u(y),$$

so that $f(x,y)$ may be sampled by drawing two independent uniform random variables, ξ_i,η_i and forming the estimator, G_2, which sums up the number of times $\xi_i^2 + \eta_i^2 \leq 1$. An algorithm for performing the Monte Carlo integration in pseudocode is

```
Initialize sum = 0
Repeat N times, i = 1, ..., N
    x = rand(u)
    y = rand(u)
    If(x^2 + y^2 <= 1.0) then
       sum = sum + 1
    EndIf
EndRepeat
mean = sum/N
```

The two methods are of comparable effectiveness. Of course, neither is a method of choice for this or other one-dimensional integrals. Which of the two estimators, G_1 or G_2, will be used in actual practice depends on factors such as the variance and efficiency of the calculation.

But a seemingly paradoxical outcome is seen: an integral in one dimension is recast as an integral in two without serious, if any, loss of computational efficiency. That one can work in many dimensions – indeed one can add extra dimensions – is a characteristic of Monte Carlo quadrature in contrast to discrete numerical quadrature, and is a property that can be exploited to great advantage in many applications.

The procedure detailed above may be easily generalized. To evaluate the L-dimensional integral over the unit hypercube

$$\int \cdots \int g(x_1, x_2, \ldots, x_L)\, \mathrm{d}x_1\, \mathrm{d}x_2 \ldots \mathrm{d}x_L,$$

L uniform random variables could be sampled, the function $g(x_1, x_2, \ldots, x_L)$ calculated, and the whole process repeated N times. The arithmetic mean of the function values gives an unbiased estimate of the integral.

Of course, given the ability to generate random variables from any distribution over any space (as discussed in the next chapter) the domain of integration need not be limited to hypercubes.

When a variable is generated using rand(u) or a similar function, it is a pseudorandom variable; that is, it was generated by a deterministic algorithm.

Since it is possible to use truly random variables in any calculation, why are pseudorandom variables used? An absolute requirement in debugging a computer code is the ability to repeat a particular run of the program. If truly random numbers were used, an identical calculation could not be repeated and the recurrence of an error would be left to chance. It has been suggested that pseudorandom numbers be used to debug a program and that in the actual exercising of the program truly random numbers be used. This method also suffers from the inability to repeat a particular calculation. If after many hours of computer time an error should occur in a code (subtle logical errors occur in many Monte Carlo codes), it is of utmost importance to be able to repeat the error at will as an aid to debugging. It is also very useful to be able to repeat a calculation when changes are made or when the program is moved to a different computer. Furthermore, lengthy calculations may require the generation of an enormous number of ''random variables'' at great rates, and deterministic algorithms can be created to fill this need. The generation of pseudorandom variables is discussed in much greater detail in Chapter 9.

Finally, there are situations in which the same sequence of random variables must be generated, for example, to change a parameter but retain the correlation with a previous calculation. In that case, the use of pseudorandom sequences offers a great advantage.

2.10 Monte Carlo Estimators

We have defined an estimator as a useful approximation to a quantity of interest Q, which may be derived from a Monte Carlo calculation. In the example given in Equations 2.48 and 2.49 in which

$$\frac{\pi}{4} = \int \sqrt{1-x^2}\,\mathrm{d}x \approx \frac{1}{N}\sum_i \sqrt{1-\xi_i^2},$$

we consider Q to be $\frac{\pi}{4}$ and our estimator is the approximation on the right-hand side, which is a function $\theta(\xi_1, \xi_2, \ldots, \xi_N)$ of the N random or pseudorandom variables used in the calculation.

The function θ is of course itself random, and the statement that it gives a satisfactory approximation to Q means that it is not expected to fluctuate far from Q. Put a little more formally,

$$\langle(\theta - Q)^2\rangle/Q^2 \ll 1.$$

Acceptable values of the ratio depend on the application. A Monte Carlo calculation may be intended to give a rough estimate of some numerical quantity, or it may be aimed at high precision, or at a target in between. The appropriate balance between small or zero bias and small variance will depend on these choices.

We write

$$\langle(\theta - Q)^2\rangle = \langle(\theta - \langle\theta\rangle)^2\rangle + (\langle\theta\rangle - Q)^2$$

and observe that the quality of θ as a measure of Q comes separately from the variance of θ and from the departure of its mean from Q. The quantity $\langle\theta\rangle - Q$ is called the *bias of the estimator*. An unbiased estimator is one for which $\langle\theta\rangle = Q$ for any experiment whatever the number N may be.

The quadratures we have discussed are unbiased since the result is linear in the functions calculated. For some problems, however, it is very difficult to formulate unbiased estimators. As we shall see, there are many problems for which the answer required is a ratio of integrals,

$$Q = \frac{\int_0^1 g_1(x)\,\mathrm{d}x}{\int_0^1 g_2(x)\,\mathrm{d}x},$$

for which a suitable estimator is

$$\theta(\xi_1, \ldots, \xi_N) = \frac{\sum_i g_1(\xi_i)}{\sum_i g_2(\xi_i)}.$$

Since this is not a linear function of g_2, it is biased. An example that can easily be analyzed is

$$1 = \frac{1}{\int_0^\infty x e^{-x}\,\mathrm{d}x} \approx \frac{N}{\sum_{i=1}^N (-\log(\xi_i))}.$$

The random variable X is sampled from an exponential distribution (see Section 3.1) and an estimator for the quotient is formed. It can then be shown that

$$\left\langle \frac{N}{\sum(-\log \xi_i)} \right\rangle = \frac{N}{N-1} \to 1 + \frac{1}{N} + \frac{1}{N^2} + \cdots.$$

Our estimator is biased by $\frac{1}{N}$, which, for large N, decreases faster than the standard error of the mean ($\sigma/\sqrt{N}$); where here $\sigma = 1$. This $\frac{1}{N}$ behavior is typical of the bias of such ratios. The results that may be derived from a Monte Carlo calculation are more general than this, and may have different variation of the bias. It is of course best if the bias becomes 0 as N grows large.

An estimator θ is termed *consistent* for the quantity Q if θ converges to Q with probability 1 as N approaches infinity. That is, θ is a consistent estimator of Q if

$$P\{\lim_{N\to\infty} \theta(\xi_1, \xi_2, \ldots, \xi_N) = Q\} = 1.$$

The law of large numbers states that the sample mean $\overline{X}_N$ is a consistent (and unbiased) estimator of the mean μ. It further implies that estimators of quotients that are quotients of means are also consistent (although, in general, biased).

While unbiased estimators are desirable, they should not be introduced at the expense of a large variance, since the overall quality is a combination of both bias and consistency. In general, one seeks the minimum of $\langle(\theta - Q)^2\rangle$.

An example may clarify the issue. Suppose $\{\xi_i\}$ are drawn uniformly and independently on the interval $(0, 1)$ and we wish to estimate the mean, Q, from the chosen ξ_i. The estimator

$$\overline{X}_N = \theta_1 = \frac{1}{N}\sum \xi_i.$$

is the usual one discussed above. A plausible alternative for large N is

$$\theta_2 = \frac{1}{2}\max(\xi_1, \xi_2, \ldots, \xi_N).$$

Note that this estimator always gives results less than the mean, $\frac{1}{2}$. It is easy to show that

$$E(\theta_1) = Q = \frac{1}{2},$$
$$\text{var}\{\theta_1\} = \frac{1}{12N} = O\left(\frac{1}{N}\right),$$

while

$$E(\theta_2) = \frac{N}{N+1}Q = Q\left(1 + O\left(\frac{1}{N}\right)\right),$$
$$E(\theta_2 - Q)^2 = \frac{2Q^2}{(N+1)(N+2)} = O\left(\frac{2}{N^2}\right).$$

Thus, although θ_2 is biased (by $\frac{2}{N}$), its variance for large N is smaller than that of θ_1 by a ratio of $\frac{N}{3}$. The bias is then equal to its standard deviation. For some purposes, this would be a more useful estimator.

Just as a good Monte Carlo calculation must be supplemented with an estimate of the statistical error, sources of bias should be identified. The bias should be estimated numerically or an upper bound should be determined. A useful way of estimating bias when the behavior with N is known is to group the data in samples smaller than N, say $n = N/m$. One can average this more biased estimator over the m groups obtained and study the dependence on m:

$$\text{Bias of } \frac{\sum_{i=1}^{N} g_1(\xi_i)}{\sum_{i=1}^{N} g_2(\xi_i)} \approx \frac{c}{N},$$

$$\text{Bias of } \frac{1}{m}\sum_{l=1}^{m}\left(\frac{\sum_{i=n(l-1)+1}^{nl} g_1(\xi_i)}{\sum_{i=n(l-1)+1}^{nl} g_2(\xi_i)}\right)_{\text{group}_l} = \frac{c}{n} = \frac{cm}{N}.$$

with c being a positive constant.

We note in passing that this method of grouping is also a practical way of estimating the variance of the quotient. This consists in selecting groups of numerators and denominators that are nearly independent, forming partial quotients for the groups, and then applying Equation 2.44.

References

1 Kac, M. (**1983**) What is random? *American Scientist*, **71**, 405.
2 Kirschenmann, P. (**1972**) Concepts of randomness. *Journal of Philosophical Logic*, **1**, 395.
3 Cramér, H. (**1946**) *Mathematical Methods of Statistics*, Princeton University Press, Princeton, pp. 137–44; paperback, 1999.
4 Doob, J.L. (**1953**) *Stochastic Processes*, John Wiley & Sons, Ltd, New York. Expectation Values are discussed on pp. 12 and 13. Equality of the two definitions is proved on pp. 617–22.
5 Révész, P. (**1968**) *The Laws of Large Numbers*, Academic Press, New York.

Further Reading

Elementary

Chung, K.L. (**1979**) *Elementary Probability Theory with Stochastic Processes*, Springer-Verlag, New York.
Cramér, H. (**1958**) *The Elements of Probability Theory*, John Wiley & Sons, Ltd, New York.

More Advanced

Cramér, H. (**1970**) *Random Variables and Probability Distributions*, Cambridge University Press, London; paperback, 2004.
Feller, W. (**1950**) *An Introduction to Probability Theory and Its Applications*, Vols. 1 and 2, John Wiley & Sons, Ltd, New York.

3
Sampling Random Variables

We have sketched how a Monte Carlo calculation is a numerical stochastic process. The next step consists in designing and carrying out such a process so that answers to interesting questions may be obtained. In doing so, it is usually required that random variables be drawn from distribution functions that define the process. For example, to evaluate the integral $\int f(x)g(x)\,\mathrm{d}x$, values of X must be drawn from $f(x)$ and the average value of $g(x)$ over a set of such X calculated. The process of "sampling X from $f(x)$," as it is ordinarily called, is therefore an essential technical matter. It is the purpose of this chapter to introduce the reader to the methods required. It will be beyond our scope to give a complete review or survey of methods or of known algorithms. References will be supplied to other literature [1, 2]. Our treatment may serve to illustrate important principles, to exercise ideas of probability, but above all to demonstrate that sampling any $f(x)$ can in fact be carried out. At the same time, some specific techniques and results will be presented. First, we must define what we mean by *sampling*. Consider some space Ω_0 and $x \in \Omega_0$, together with a probability distribution function[1)] $f(x)$, where

$$\int_{\Omega_0} f(x)\,\mathrm{d}x = 1.$$

A sampling procedure is an algorithm that can produce a sequence of values of X ("random variables") $X_1, X_2, \ldots$ such that for any $\Omega \in \Omega_0$

$$P\{X_k \in \Omega\} = \int_{\Omega} f(x)\,\mathrm{d}x \leq 1. \tag{3.1}$$

For a one-dimensional distribution defined on $(0, 1)$, this means that

$$P\{X_k \in (a, b)\} = \int_a^b f(x)\,\mathrm{d}x, \quad 0 < a < b < 1.$$

Informally, for small values of $b - a = \mathrm{d}x$,

$$P\{X_k \in \mathrm{d}x\} = f(x)\,\mathrm{d}x.$$

1) The case in which the space is discrete, and the case of mixed discrete and continuous variables need only a slight change of notation.

Monte Carlo Methods. Second Edition. M.H. Kalos and P.A. Whitlock

ISBN: 978-3-527-40760-6

It will be possible to do this only by already having a sequence of some basic random variables. It has become conventional to start with random variables that are independent and uniformly distributed on (0, 1). We shall denote these by $\xi_1, \xi_2, \ldots$, and assume that they can be generated by a computer procedure called rand(u). Such routines are widely available and usually giving satisfactory imitations of truly random variables. These are called *pseudorandom numbers*. It is important to note that here *satisfactory* means that the results are adequate in a particular context. No general method has ever been proved acceptable in any but the most elementary calculations, and well-known computer manufacturers have supplied bad pseudorandom generators. It is unfortunately necessary to test such generators both intrinsically and in the context of a specific class of applications. Further discussion of these issues is given in Chapter 9. However, in the discussion that follows, an indefinite supply of uniform pseudorandom variables is assumed to exist.

3.1 Transformation of Random Variables

Suppose that X is a random variable with cumulative distribution function $F_X(x)$ and pdf,

$$f_X(x) = \frac{\mathrm{d}F_X}{\mathrm{d}x},$$

and that the random variable $Y = y(X)$ is a continuous nondecreasing function of x as in Figure 3.1. What is $F_Y(y)$? The variable X and the function $y(X)$ map into each other

$$y(X) \leq y(x) \quad \text{iff} \quad X \leq x, \tag{3.2}$$

so the probabilities become

$$P\{y(X) = Y \leq y(x)\} = P\{X \leq x\} \tag{3.3}$$

or

$$F_Y(y) = F_X(x). \tag{3.4}$$

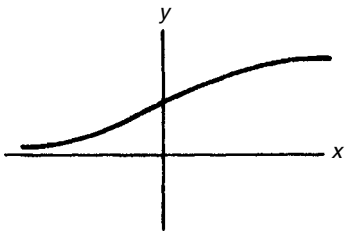


Figure 3.1 y is a continuous nondecreasing function of x.

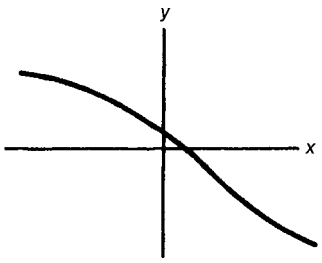


Figure 3.2 y is a nonincreasing function of x.

The relationship between the probability distribution functions may be determined by differentiating Equation 3.4:

$$f_Y(y)\frac{dy}{dx} = f_X(x). \tag{3.5}$$

Suppose that $y(X)$ is a nonincreasing function of X (Figure 3.2); then

$$P\{y(X) \leq y(x)\} = P\{X \geq x\} = 1 - P\{X < x\}, \tag{3.6}$$

since

$$P\{X \geq x\} + P\{X < x\} = 1. \tag{3.7}$$

The cumulative distribution function for Y is, therefore,

$$F_Y(y) = 1 - F_X(x) \tag{3.8}$$

and

$$f_Y(y)\frac{dy}{dx} = -f_X(x). \tag{3.9}$$

The probabilities in Equation 3.9 are nonnegative since dy/dx is negative. The relationship between the pdf's of X and Y for both cases can be combined in one equation as

$$f_Y(y)\left|\frac{dy}{dx}\right| = f_X(x). \tag{3.10}$$

Thus, given that X is a random variable with pdf $f_X(x)$ and $Y = y(X)$, then

$$f_Y(y) = f_X(x)\left|\frac{dx}{dy}\right| = f_X(x)\left|\frac{dy}{dx}\right|^{-1}. \tag{3.11}$$

Equation 3.11 is also written as

$$|f_X(x)\,dx| = |f_Y(y)\,dy|, \tag{3.12}$$

reflecting the fact that all the values of X in dx map into values of Y in dy (Figure 3.3). We now give some simple examples.

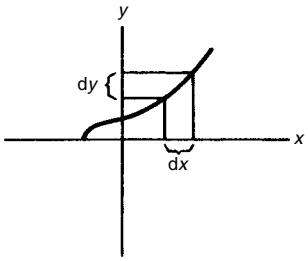


Figure 3.3 Values of X in dx map into values of Y in dy.

Suppose that X is a random variable on $(0, 1)$ with

$$f_X(x) = \frac{4}{\pi}\frac{1}{1+x^2}, \quad 0 \le x < 1 \tag{3.13}$$

and $Y = 1/X, 1 < Y < \infty$, then

$$\frac{dy}{dx} = -\frac{1}{x^2} = -y^2$$

and

$$f_Y(y) = \left(\frac{4}{\pi}\right)\frac{1}{1+x^2}y^{-2} = \left(\frac{4}{\pi}\right)\frac{1}{1+1/y^2}\frac{1}{y^2} = \left(\frac{4}{\pi}\right)\frac{1}{1+y^2}. \tag{3.14}$$

The pdf $f_Y(y)$ is a different distribution; however, in this case, it has the same functional form as $f_X(x)$, but on a different domain.

As another example, consider the linear transformation $Y = a + bX$. Now

$$f_Y(y) = |b^{-1}| f_X\left(\frac{y-a}{b}\right). \tag{3.15}$$

In particular, let $f_X(x) = 1$ for X on $[0, 1]$; then

$$f_Y(y) = \begin{cases} b^{-1}, & a \le y \le a+b \text{ for } b > 0 \\ -b^{-1}, & a+b \le y \le a \text{ for } b < 0. \end{cases} \tag{3.16}$$

Equation 3.15 can be used to prove a relation asserted in Section 2.8. The characteristic function of $y(x)$ is

$$c_Y(t) = \int_{-\infty}^{\infty} e^{iyt} f_Y(y)\, dy = b^{-1}\int_{-\infty}^{\infty} e^{iyt} f_X\left(\frac{y-a}{b}\right) dy. \tag{3.17}$$

By changing variables $u = (y - a)/b$, the integral becomes

$$c_Y(t) = \int_{-\infty}^{\infty} e^{i(a+bu)t} f_X(u)\, du = e^{iat} c_X(bt). \tag{3.18}$$

For the case when $a = 0$ and $b = 1/n$, Equation 3.18 reduces to

$$c_Y(t) = c_X\left(\frac{t}{n}\right). \tag{3.19}$$

Suppose X is distributed normally with mean 0 and variance 1:

$$f_X(x) = \phi'(x|0,1) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{x^2}{2}\right], \quad -\infty < x < \infty, \tag{3.20}$$

and Y is a linear transformation of X, $Y = \sigma X + \mu$. Then

$$f_Y(y) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left[-\frac{1}{2}\left(\frac{y-\mu}{\sigma}\right)^2\right]. \tag{3.21}$$

The random variable Y is also normally distributed, but its distribution function is centered on μ and has variance σ^2.

In the discussion, so far we have talked about transforming a random variable X having any distribution into a random variable Y. Because conventional pseudorandom number generators yield values uniform on $(0,1)$, the transformation from that case is particularly important and is also called *inversion*. The pdf for a uniform random variable on $(0,1)$ is

$$f_\xi(\xi) = \begin{cases} 0 & \text{for } \xi < 0 \text{ or } \xi > 1 \\ 1 & \text{otherwise.} \end{cases} \tag{3.22}$$

Now consider as an example the family of functions

$$Y = \xi^r. \tag{3.23}$$

Then the probability distribution function for Y is

$$f_Y(y) = \left|\frac{1}{r}\right| y^{1/r-1} \begin{cases} 0 < y < 1 & \text{if } r > 0 \\ 1 < y < \infty & \text{if } r < 0. \end{cases} \tag{3.24}$$

If $r > 1$, the power of Y will be negative, for example,

$$r = 2 \Rightarrow f_Y(y) = \tfrac{1}{2} y^{-\frac{1}{2}}.$$

This pdf diverges at the origin; distributions can be singular. As $r \to \infty$, the pdf becomes arbitrarily close to $f_Y(y) = y^{-1}$, but never reaches it since $f_Y(y)$ must be integrable. If it is necessary to sample a power law, Equation 3.24, on $0 < y < 1$ or $y > 1$, then the transformation given above, Equation 3.23, may be used. The functions in Equation 3.24 will also be useful in evaluating integrals of singular functions by sampling singular pdf's. What is meant by this will be explained more fully in Chapter 4.

Another useful transformation is

$$Y = -\log \xi, \quad Y \text{ on } (0,\infty). \tag{3.25}$$

The transformation can be written $\xi = e^{-Y}$ so that the pdf for y is

$$f_Y(y) = f_\xi(\xi) \left|\frac{d\xi}{dy}\right|^{-1}, \qquad \left|\frac{d\xi}{dy}\right| = \frac{1}{\xi} = e^y,$$

so finally

$$f_Y(y) = e^{-y}. \tag{3.26}$$

That is, the random variable, which is the natural logarithm of a uniform random variable, is distributed exponentially.

Specific Algorithms

We now consider the problem of finding an algorithm to sample a specified function. This is usually the form in which the problem is posed. For univariate distributions, there is a general inversion technique that may be justified as follows.

Let $Y = y(X)$ be an increasing function of X. The cumulative distribution function of Y may be determined from Equation 3.4. If $X = \xi$ is uniform, its cumulative distribution function is

$$F_\xi(\xi) = \begin{cases} 0, & \xi < 0 \\ \xi, & 0 \le \xi \le 1 \\ 1, & \xi \ge 1. \end{cases} \tag{3.27}$$

Therefore, on $(0, 1)$ the cumulative distribution function for Y is determined by solving the equation

$$F_Y(y) = \xi \qquad \text{for } Y. \tag{3.28}$$

Sampling an Exponential

Suppose the pdf for Y is given by

$$f_Y(y) = \lambda e^{-\lambda y}, \quad 0 < y < \infty, \tag{3.29}$$

which is a generalization of Equation 3.26. Then from Equations 3.28 and 3.29

$$F_Y(y) = \int_0^y \lambda e^{-\lambda u} du = 1 - e^{-\lambda y} = \xi. \tag{3.30}$$

which yields

$$Y = -\frac{1}{\lambda} \log(1 - \xi), \tag{3.31}$$

an increasing function of ξ. The expression in Equation 3.31 is computationally equivalent[2] to $-(1/\lambda)\log(\xi)$. This is true since, if ξ is uniform on $(0, 1)$, then $1 - \xi$ is also uniform on $(0, 1)$. The decision about which form to use depends both on whether $f_Y(y)$ is increasing or decreasing and on convenience.

Sampling $\frac{2}{\pi}\frac{1}{1+y^2}$

As another example, let

$$f_Y(y) = \frac{2}{\pi}\frac{1}{1+y^2}, \quad 0 < y < \infty; \tag{3.32}$$

2) By computationally equivalent we do not mean that the value of Y is the same in both cases. Rather, the distributions are the same and both give statistically equivalent results when used in a Monte Carlo calculation.

then the cumulative distribution function is

$$F_Y(y) = \int_0^y \frac{2}{\pi}\frac{1}{1+u^2}\,du = \frac{2}{\pi}\tan^{-1} y = \xi.$$

Solving this equation for Y yields

$$Y = \tan\frac{\pi}{2}\xi. \tag{3.33}$$

If a random variable Y is required having pdf $[\pi(1+y^2)]^{-1}$ on $(-\infty, \infty)$, this may be accomplished by assigning a sign to Y randomly,

$$\text{if } \xi_1 < \tfrac{1}{2}, \quad Y = -\tan\tfrac{\pi}{2}\xi_2,$$

$$\text{if } \xi_1 > \tfrac{1}{2}, \quad Y = +\tan\tfrac{\pi}{2}\xi_2.$$

It is left to the reader to show that if the pdf of Y is

$$f_Y(y) = \frac{1}{\pi}\frac{1}{1+y^2}, \quad -\infty < y < \infty,$$

then Y may be obtained from the transformation

$$Y = \tan\frac{\pi}{2}(2\xi - 1).$$

Sampling $r\exp(-\frac{1}{2}r^2)$

A useful pdf is

$$f_R(r) = r\exp\left[-\frac{1}{2}r^2\right], \quad 0 < r < \infty, \tag{3.34}$$

whose cumulative distribution function is given by

$$F_R(r) = \int_0^r u\exp\left[-\frac{1}{2}u^2\right]du = 1 - \exp\left[-\frac{1}{2}r^2\right] = \xi.$$

A random variable that is distributed as in Equation 3.34 is then

$$R = [-2\log(1-\xi)]^{\frac{1}{2}}.$$

which is computationally equivalent to

$$R = [-2\log\xi]^{\frac{1}{2}}. \tag{3.35}$$

The Box–Muller Method for Sampling a Gaussian or Normal Distribution

It is frequently necessary to sample a Gaussian,

$$\phi'(y|0,1) = \frac{1}{\sqrt{2\pi}}\exp\left[-\frac{1}{2}y^2\right], \quad -\infty < y < \infty, \tag{3.36}$$

in Monte Carlo calculations. In practice, it is easier to sample two independent Gaussian random variables, Y_1 and Y_2, together, than to sample a single variable:

$$f(y_1, y_2) = \phi'(y_1|0,1)\,\phi'(y_2|0,1) = \frac{1}{2\pi}\exp\left[-\frac{1}{2}\left(y_1^2 + y_2^2\right)\right].$$

Now, the equation can be transformed into the independent polar coordinates R and Φ by the transformation

$$Y_1 = R\cos\Phi,$$

$$Y_2 = R\sin\Phi,$$

and rewritten as

$$\phi'(y_1)\phi'(y_2)\,\mathrm{d}y_1\,\mathrm{d}y_2 = \left(\exp\left[-\frac{1}{2}r^2\right] r\,\mathrm{d}r\right)\left(\frac{1}{2\pi}\,\mathrm{d}\phi\right). \tag{3.37}$$

The angle Φ is distributed uniformly on $(0, 2\pi)$ and may be sampled by

$$\Phi = 2\pi\xi_2.$$

The probability distribution function for R is the same as that introduced in Equation 3.34, so R can be sampled as in Equation 3.35. The two independent Gaussian random variables become

$$Y_1 = [-2\log\xi_1]^{\frac{1}{2}}\cos 2\pi\xi_2,$$

$$Y_2 = [-2\log\xi_1]^{\frac{1}{2}}\sin 2\pi\xi_2; \tag{3.38}$$

this is known as the *Box–Muller* method (though it was invented by Wiener [3]). The equations can be linearly transformed to any μ and any σ as described above (see Equation 3.21). A good function may be programmed using the Box–Muller method; however, as written the method is convenient but slow. One advantage is that it permits the sampling of a gaussian random variable in one coded expression.

Approximate Gaussian Sampling

An approximate Gaussian random variable may also be generated by invoking the central limit theorem. By sampling N uniform random variables $\xi_1, \xi_2, \ldots, \xi_N$ and forming the sum

$$Y = \sqrt{12/N}\left(\sum_{k=1}^{N}\xi_k - \frac{N}{2}\right), \tag{3.39}$$

a variable with mean 0 and variance 1 is generated. The central limit theorem asserts that this will be nearly gaussian for large N. A value of $N = 12$ appears to be sufficiently large for many purposes and avoids the evaluation of the factor $\sqrt{12/N}$.

3.2 Numerical Transformation

In the preceding examples, an expression for sampling a random variable was derived by applying

$$F_Y(y) = \xi.$$

This equation can always be used if $y(\xi)$ is an increasing function, but in practice solving it may require a slow iteration procedure. For example, a transcendental equation must be solved anew for each value of ξ.

An attempt to generate a Gaussian random variable by the equation

$$\phi(x|0,1) = \xi$$

requires solving the expression for the error function,

$$\frac{1}{\sqrt{2\pi}} \int_0^x \exp\left[-\frac{u^2}{2}\right] du = \operatorname{erf}(x) = \xi,$$

for X. The method of setting a uniform random variable equal to the cumulative distribution function is useful only if the resulting equation is economically solvable. Finally, it may be that $f(y)$ is known only numerically (e.g. from experimental data).

A general, straightforward, and economical approximation to the required inversion may be obtained if the specific values of the cumulative distribution function for Y can be computed in advance. That is, let

$$F(y_n) = \int_0^{y_n} f_Y(y)\, dy = \frac{n}{N}, \quad n = 0, 1, 2, \ldots, N, \tag{3.40}$$

where $y_0 = 0$. As before, we must solve

$$F(y) = \xi$$

for Y. Find n such that

$$\frac{n}{N} < \xi < \frac{n+1}{N}.$$

The value for Y may be calculated by linear interpolation

$$Y = y_n + (y_{n+1} - y_n)u, \tag{3.41}$$

where

$$u = N\xi - n, \quad 0 < u < 1.$$

This method corresponds to approximating a pdf by a piecewise-constant function with the area of each piece a fixed fraction as in Figure 3.4. It is most accurate when the pdf is large and is least accurate when the pdf is small. Rather than linearly interpolating, the value of Y may simply be set to the nearest y_n. This approximates the original $f_Y(y)$ as a discrete distribution.

3.3 Sampling Discrete Distributions

According to Equation 3.22 the distribution function for a uniform random variable is

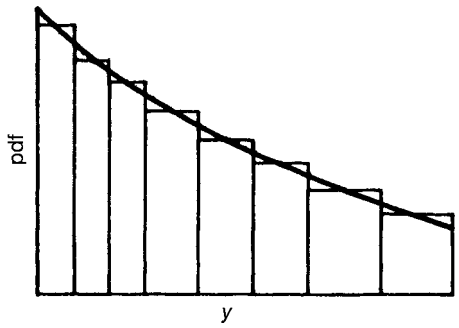


Figure 3.4 Approximating a numerical $f(y)$ by a piecewise-constant function.

$$f_\xi(\xi) = 1, \quad 0 \le x \le 1.$$

Using Equation 2.21, we have that

$$P\{0 \le x_1 < \xi \le x_2 \le 1\} = F_\xi(x_2) - F_\xi(x_1) = x_2 - x_1. \tag{3.42}$$

The chance that ξ lies in an interval $[x_1, x_2]$ of $(0, 1)$ is equal to the length of the interval. Suppose we have a class of events E_k with probabilities f_k and we wish to sample one at random. We may generate a uniform variable ξ and, if it lies in an interval of length f_k on $(0, 1)$, assign event k to that trial. Better, since $\sum f_k = 1$, it is possible to take the interval $(0, 1)$ and exhaust it by dividing it into segments each of which has a length equal to some f_l (Figure 3.5). The interval into which a ξ falls determines the identity of the event.

A uniform random variable is generated, and the smallest l is found for which the sum of the f_k is greater than the random number; that is,

$$\sum_{k=0}^{l-1} f_k < \xi \le \sum_{k=0}^{l} f_k. \tag{3.43}$$

(When $l = 0$, the sum is defined to equal 0.) Whenever $0 < \xi < f_1$, event 1 takes place; if $f_1 < \xi < f_1 + f_2$, event 2 takes place; and so on.

Thus, if we must choose between equally likely events, we may consider the first to be selected if some $\xi < \frac{1}{2}$ otherwise, the second is selected. To select three events with probabilities $\frac{1}{2}, \frac{1}{4}$, and $\frac{1}{4}$, we choose the first if $\xi < \frac{1}{2}$, the second if $\xi < \frac{3}{4}$, and the third otherwise.

Suppose we must choose among K equally likely events,

$$f_k = \frac{1}{K}, \quad k = 1, 2, \ldots, K.$$

Figure 3.5 Dividing the interval $(0, 1)$ into segments of length f_l.

The sums in Equation 3.43 are formed and reduced to

$$\frac{l-1}{K} < \xi \leq \frac{l}{K},$$

$$l - 1 < \xi K \leq l.$$

The appropriate value of l for a particular ξ is then

$$l = [\xi K] + 1,$$

where $[u]$ indicates truncation to the largest integer less than u.

In searching for an index l satisfying Equation 3.43, a binary search is strongly recommended when the total number of intervals is large and if $\sum f_k$ does not converge fast. If a serial search is to be used and the index can be arranged at our disposal, then the index with the largest probability should be put in the first place, and so on, to reduce the average time of searching.

The Geometric Distribution

An illustration of efficient searching is found in sampling the geometric distribution

$$f_k = 2^{-k}, \quad k = 1, 2, \ldots.$$

The procedure starts with the largest probability:

```
Initialize fk = 0.5
Initialize x = rand(u)
Repeat Until x <= fk, k = 1, ...
    fk = 0.5*fk
    k = k + 1
EndRepeat
K = k
```

Since the probabilities decrease, the chances are good that the loop terminates quickly. In fact, two tests are required, on the average, before it does. Alternatively, it is possible to sample K directly (i.e. by solving Equation 3.43 explicitly) to get in pseudocode

$$K = -log(rand(u))/log(2) + 1.$$

The decision on which method to use to sample the geometric distribution depends on the computer used. If evaluation of logarithms is slow, it is better to use the multiplicative method shown first.

On the other hand, for sampling

$$f_k = (1 - \alpha)\alpha^{k-1}; \quad k = 1, 2, \ldots,$$

the expected number of passes through a loop as in the pseudocode given above is $1/(1-\alpha)$, which is large for α close to 1. A binary search can be carried out in time proportional to $-\log(1-\alpha)$, but the computation by way of $-\log(\xi)/\log(\alpha)$ takes constant time.

Further illustrations of the sampling of discrete distributions will be given in the discussion of other methods. In particular, the composition method (Section 3.4) involves sampling discrete marginal distributions and continuous (or discrete) conditional distributions.

Mixed Distributions

A mixed distribution has a cumulative distribution function that is partly continuous, but with step discontinuities. An example is shown in Figure 3.6. It may be sampled by mapping if care is taken to map ξ to the appropriate part of $F_X(x)$.

Consider

$$F_X(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 - \frac{1}{2}e^{-\lambda x} & \text{for } x > 0. \end{cases} \tag{3.44}$$

The step of $\frac{1}{2}$ at $x = 0$ indicates that the discrete value $x = 0$ occurs with probability $\frac{1}{2}$; values of $x > 0$ are distributed continuously from zero to infinity. Negative values of x never occur. To sample this, we select ξ and set

$$X = \begin{cases} 0 & \text{if } \xi \le \frac{1}{2} \\ -\log(2(1-\xi))/\lambda & \text{otherwise.} \end{cases} \tag{3.45}$$

That is, we solve $F_X(x) = \xi$ when $\xi > \frac{1}{2}$.

In summary, suppose that $Y = y(X)$ is a discrete random variable. A value of Y is sampled by generating a uniform random variable and deciding what value of Y contains ξ in its range:

$P\{\xi \text{ in a particular range}\} = \text{length of discrete segment.}$

This procedure is demonstrated in Equation 3.43. If the cumulative distribution function also contains continuous sections, Equation 3.28 must be solved in these sections.

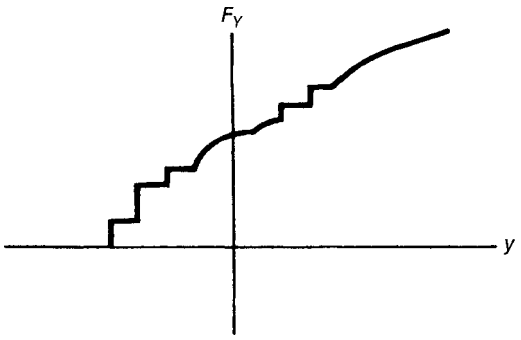


Figure 3.6 A mixed distribution function.

3.4
Composition of Random Variables

We have indicated that transforming or inversion of random variables may lead to unpleasantly complicated equations to solve numerically. Another technique for generating random variables having a required distribution is to take two or more different (usually independent) random variables drawn from known distributions and combine them in interesting ways. The Box–Muller method of Equation 3.38 is in fact an example of sampling by composition. The simplest example is to simply add two independent random variables.

3.4.1
Sampling the Sum of Two Uniform Random Variables

Let X and Y be uniform on $(0, 1)$ and $Z = X + Y$; then

$$F_Z(z) = P\{X + Y < z\} \tag{3.46}$$

is the area under the line $Z = X + Y$ within the unit square as shown in Figure 3.7.

Consider the case where $X + Y < 1$. Geometrically, $F_Z(z)$ is seen (Figure 3.8) to be the area of the triangle with sides equaling z:

$$F_Z(z) = \tfrac{1}{2}z^2.$$

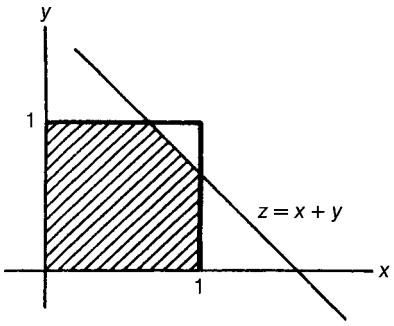


Figure 3.7 The sum of two random variables.

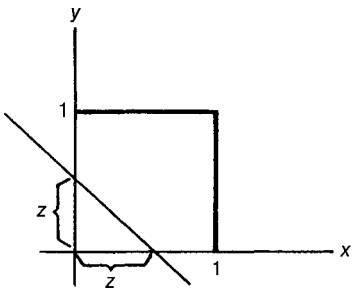


Figure 3.8 $F_Z(z)$ when $X + Y < 1$.

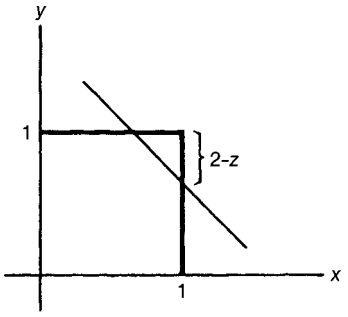


Figure 3.9 $F_Z(z)$ when $X + Y > 1$.

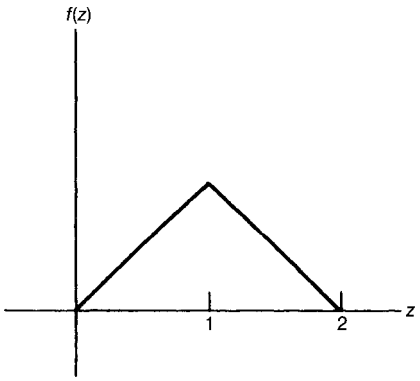


Figure 3.10 The probability distribution function $z = x + y$.

For $X + Y > 1$ (refer to Figure 3.9), the cumulative distribution function is

$$F_Z(z) = 1 - \tfrac{1}{2}(2 - z)^2.$$

The corresponding pdf's are

$$f_Z(z) = \begin{cases} z, & 0 < z < 1 \\ 2 - z, & 1 \leq z < 2, \end{cases} \tag{3.47}$$

which when taken together gives the pdf in Figure 3.10. It is left as an exercise for the reader to find the pdf when two uniform random variables are multiplied.

3.4.2 Sampling a Random Variable Raised to a Power

Another form of composition is illustrated as follows. Let $X_1, X_2, \ldots, X_n$ be drawn independently from the cumulative distribution functions $F_1(x_1), F_2(x_2), \ldots, F_n(x_n)$. Set Z to be the largest of the X_i,

$$Z = \max\{X_1, X_2, \ldots, X_n\}. \tag{3.48}$$

What is the distribution function? The following statement holds:

$$Z = \max\{X_1, X_2, \ldots, X_n\} \leq z \tag{3.49}$$

if and only if

$$X_1 \leq z \text{ and } X_2 \leq z \text{ and } \ldots \text{ and } X_n \leq z.$$

Since the X_i are all independently distributed,

$$P\{Z \leq z\} = P\{X_1 \leq z\}P\{X_2 \leq z\} \ldots P\{X_n \leq z\}$$

or

$$P\{Z \leq z\} = \prod_{i=1}^{n} F_i(z). \tag{3.50}$$

A similar proof holds for the smallest of n random variables.

Suppose z equals the maximum of k uniform random variables

$$Z = \max\{\xi_1, \xi_2, \ldots, \xi_k\}; \tag{3.51}$$

then

$$F_Z(z) = \prod_{i=1}^{k} F_i(z) = z^k \tag{3.52}$$

since

$$F_i(\xi) = \xi$$

for a uniform random variable. The pdf corresponding to $F_z(z)$ is

$$f(z) = kz^{k-1}, \quad 0 < z < 1. \tag{3.53}$$

The algorithm for Equation 3.51 in pseudocode is

```
Initialize z = 0.0
Repeat k times, ik = 1, ..., k
    z = max(rand(u), z)
    ik = ik + 1
EndRepeat
```

It is also possible to sample a Z by transformation:

$$F_Z(z) = z^k = \xi,$$
$$Z = \xi^{1/k}, \tag{3.54}$$

which in pseudocode is written as follows:

```
z = rand(u) ^(1./k).
```

In a computer calculation, which method will be more efficient? Though the sampling method in Equation 3.54 may be written in one line of code, the statement invokes a logarithm and an exponential for the actual computation. Therefore, method (3.51) is faster for small values of k. As the value of k increases, more and more random numbers must be computed in the loop while the computation time of Equation 3.54 will be independent of the value of k. For larger values of k, it is preferable to employ the second method. The choice of algorithm for sampling a random variable should be guided by which is more efficient. The decision is machine and compiler dependent.

3.4.3
Sampling the Distribution $f(z) = z(1 - z)$

Let Z equal the middle value of three uniform random numbers,

$$Z = \text{mid}(\xi_1, \xi_2, \xi_3); \tag{3.55}$$

the probability distribution function for Z is then

$$f(z) = 6z(1 - z).$$

This result may be easily derived. Assume that $\xi_1 < \xi_2 < \xi_3$ so that $Z = \xi_2$. The probability that Z is in $dz = d\xi_2$ and that $\xi_1 < \xi_2$ and $\xi_3 > \xi_2$ is

$$f_Z(z)\,dz = d\xi_2 P\{\xi_1 \le \xi_2\} P\{\xi_2 \le \xi_3\} = d\xi_2 \xi_2 (1 - \xi_2) = z(1 - z)\,dz,$$

since $P\{\xi_2 \le \xi_3\} = 1 - P\{\xi_3 < \xi_2\}$. The probability that the middle value is found in any possible range $d\xi = dz$ becomes

$$\int_0^1 f_Z(z)\,dz = \int_0^1 x(1 - z)\,dz = \frac{1}{6}.$$

Taking into account the six possibilities for the arrangement of ξ_1, ξ_2, ξ_3, we get the pdf for Z

$$f(z) = 6z(1 - z). \tag{3.56}$$

The corresponding cumulative distribution function is

$$P\{\text{middle } Z < z\} = F(z) = 3z^2 - 2z^3.$$

3.4.4
Sampling the Sum of Several Arbitrary Distributions

Often a distribution function that must be sampled has (or may be written in) the form

$$f_X(x) = \sum_{i=1}^{n} \alpha_i g_i(x); \quad \alpha_i \ge 0, \quad g_i(x) \ge 0, \tag{3.57}$$

$$\int_{\Omega_0} g_i(x) \ne 1,$$

but as usual

$$\int_{\Omega_0} f_X(x)\,\mathrm{d}x = 1.$$

We now demonstrate how such a sum of terms may be sampled by random selection of a single term of the sum followed by sampling the distribution of that term. Consider a set of functions $h_i(x)$ and coefficients β_i satisfying

$$h_i(x) \geq 0, \qquad \int_{\Omega_0} h_i(x)\,\mathrm{d}x = 1,$$

$$\beta_i \geq 0, \qquad \sum_{i=1}^{n} \beta_i = 1. \tag{3.58}$$

The β_i are effectively probabilities for the choice of an event i. Let us select event m with probability β_m. Then sample X from $h_m(x)$ for that m. What is the distribution of the values of X that results? That is, what is the probability that $X \leq x$? The probability that m is chosen and $X \leq x$ is $\beta_m \int_0^x h_m(t)\,\mathrm{d}t$. Since different m are mutually exclusive, the total probability that $X \leq x$ is the sum over all m:

$$P\{X \leq x\} = \sum_{m=1}^{n} \beta_m \int_0^x h_m(t)\,\mathrm{d}t. \tag{3.59}$$

The probability distribution function that results is just

$$h(x) = \sum_{m=1}^{n} \beta_m h_m(x). \tag{3.60}$$

Again we emphasize that although a *single* $h_m(x)$ is sampled in one trial, the result, taking into account that *any* m can be used, is to sample the entire sum.

Returning to Equation 3.57, we observe that it may be rewritten as follows:

$$f_X(x) = \sum_{i=1}^{n} \alpha_i \left[\int_{\Omega_0} g_i(u)\,\mathrm{d}u\right]\left[\frac{g_i(x)}{\int g_i(w)\,\mathrm{d}w}\right]. \tag{3.61}$$

We identify

$$\beta_i = \alpha_i \int_{\Omega_0} g_i(u)\,\mathrm{d}u \tag{3.62}$$

and

$$h_i(x) = \frac{g_i(x)}{\int g_i(w)\,\mathrm{d}w}$$

and note that the conditions in Equation 3.58 are satisfied.

An example will illustrate the ideas. Consider the pdf

$$f_X(x) = \frac{3}{5}\left(1 + x + \frac{1}{2}x^2\right), \quad 0 < x < 1; \tag{3.63}$$

the sum is rewritten as

$$f_X(x) = \frac{3}{5} \times 1 + \frac{3}{5} \times \frac{1}{2} \times 2x + \frac{3}{5} \times \frac{1}{2} \times \frac{1}{3} \times 3x^2$$

so that

$$\beta_1 = \tfrac{3}{5}, \quad h_1 = 1,$$
$$\beta_2 = \tfrac{3}{10}, \quad h_2 = 2x,$$
$$\beta_3 = \tfrac{1}{10}, \quad h_3 = 3x^2,$$

and

$$\sum_{i=1}^{n=3} \beta_i = 1.$$

The value of i is chosen with probability β_i, that is,

1. sample ξ_0;
2. if $\xi_0 \leq \frac{6}{10}$, $i = 1$;
3. else if $\xi_0 \leq \frac{9}{10}$, $i = 2$;
4. else $i = 3$.

Once a value for i is selected, the appropriate h_i is sampled for X:

if $i = 1$, set $X = \xi_1$;

if $i = 2$, set $X = \max(\xi_1, \xi_2)$;

if $i = 3$, set $X = \max(\xi_1, \xi_2, \xi_3)$

since the distribution functions for X are all power laws.

Another example is the pdf

$$f_X(z) = \frac{1}{4}\left[\frac{1}{x^{\frac{1}{2}}} + \frac{1}{(1-x)^{\frac{1}{2}}}\right], \quad 0 < x < 1. \tag{3.64}$$

This may also be sampled using the algorithm suggested above by rewriting it in the form

$$f_X(x) = \frac{1}{2}\frac{1}{2x^{\frac{1}{2}}} + \frac{1}{2}\frac{1}{2(1-x)^{\frac{1}{2}}}$$

so that

$$\beta_1 = \frac{1}{2}, \qquad h_1(x) = \frac{1}{2x^{\frac{1}{2}}},$$
$$\beta_2 = \frac{1}{2}, \qquad h_2(x) = \frac{1}{2(1-x)^{\frac{1}{2}}}.$$

The cumulative distribution function corresponding to $h_1(x)$ is

$$H_1(x) = x^{\frac{1}{2}} = \xi \quad \text{or} \quad X = \xi^2;$$

similarly the cumulative distribution function corresponding to $h_2(x)$ is

$$H_2(x) = 1 - (1 - x^2)^{\frac{1}{2}} = \xi \quad \text{or} \quad X = 1 - (1 - \xi)^2.$$

But this equation may be simplified by remembering the argument that $1 - \xi$ is uniform on $(0, 1)$ if ξ is, so

$$X = 1 - \xi^2.$$

The sampling algorithm becomes

1. $X = \xi_1^2$;
2. if $\xi_2 > \frac{1}{2}$, $X = 1 - X$ $\left(\text{since } \beta_i = \frac{1}{2}\right)$. (3.65)

This is a simple method for sampling a complicated pdf.

3.5 Rejection Techniques

There is a kind of composition method that leads to very general techniques for sampling any probability distribution. It has one new feature, namely, that a trial value for a random variable is selected and proposed. This value is subjected to one or more tests (involving one or more other random variables) and it may be accepted, that is, used as needed, or rejected. If it is rejected, the cycle of choosing and testing a trial value is repeated until an acceptance takes place. An important property of the method is that the normalization of the distribution need not be known explicitly to carry out the sampling.

A disadvantage is that it may have low *efficiency*, that is, many values are rejected before one is accepted. It is an interesting technical challenge to devise efficient rejection techniques for varieties of distributions. The idea is best conveyed by a simple general case and a specific example.

Suppose we want to sample an X from a complicated pdf on $(0, 1)$, and that the "trial value" $X_0 = \xi_1$ is chosen uniformly between 0 and 1. The test to which X_0 is subjected must accept few values when $f_X(x)$ is small (near $x = 1$ in Figure 3.11) and most values when $f_X(x)$ is large (near $x = 0$). This is accomplished by accepting X_0 with probability proportional to $f_X(X_0)$. In Figure 3.11, trial values occur equally often in dx_1 and $dx_2 (= dx_1)$, but we accept a larger fraction of those in dx_1 where $f_X(x)$ is larger.

The pdf in the figure has the property that

$$f_X(x) \leq f(0). \tag{3.66}$$

A test that meets exactly our requirement that the distribution of accepted X_0 is $f_X(X_0)$ is

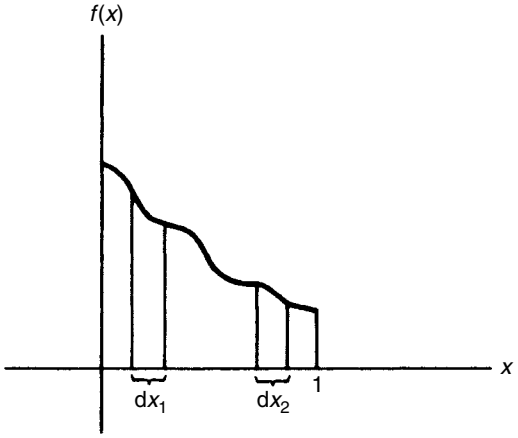


Figure 3.11 A complicated pdf that can be sampled by rejection techniques.

$$\text{Accept } X = X_0 \quad \text{if} \quad \xi_2 \leq \frac{f_X(X_0)}{f_X(0)}. \tag{3.67}$$

Stated another (geometric) way, points are chosen uniformly in the smallest rectangle that encloses the curve $f_X(x)$. The ordinate of such a point is $X_0 = \xi_1$; the abscissa is $f(0)\xi_2$. Points lying above the curve are rejected. Points below are accepted; their ordinates $X = X_0$ have distribution $f_X(x)$.

The method can be clarified by a concrete example: let

$$f_X(x) = \frac{4}{\pi}\frac{1}{1+x^2}, \quad 0 < x < 1, \tag{3.68}$$

which is a monotonically decreasing function on $(0, 1)$ (Figure 3.12).

A series of random points are generated uniformly on a rectangle enclosing $f_X(x)$. Only those points that lie below the curve $f_X(x)$ are accepted. The algorithm for accomplishing this is

1. $X_0 = \xi_1$;
2. $X_1 = \left(\frac{4}{\pi}\right)\xi_2$;
3. if $X_1 \leq \left(\frac{4}{\pi}\right)\left[\frac{1}{(1+X_0^2)}\right]$ accept $X = X_0$; otherwise repeat from step 1.

The algorithm may be rephrased more succinctly as

1. $X_0 = \xi_1$;
2. if $\xi_2 > \frac{1}{(1+X_0^2)}$, then repeat from 1; else $X = X_0$.

Or more efficiently as

1. if $\xi_2(1 + \xi_1^2) > 1$ repeat; otherwise $X = X_0 = \xi_1$.

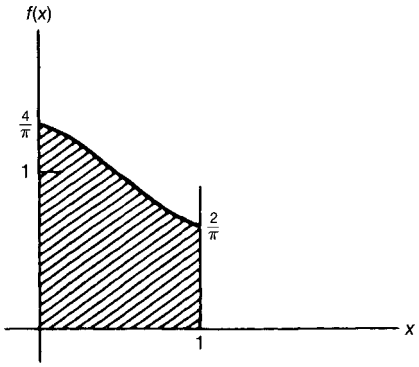


Figure 3.12 The pdf $(4/\pi)[1/(1+x^2)]$.

Let us derive the distribution function sampled in general by rejection methods. The goal is to sample an X from a pdf, $f(x)$. However, we can more easily sample a random variable Z from pdf $g(z)$. This Z is accepted, $X = Z$, with probability $h(z)$, i.e. $\xi_2 \leq h(Z) < 1$; else sample another Z. Then X has a pdf proportional to $h(z)g(z)$. Why? There are two discrete events: a success (Z is accepted, $X = Z$) and no success (Z is rejected). The joint probability that $Z < x$ and that $\xi_2 \leq h(Z)$ is

$$P\{Z < x \text{ and } \xi_2 \leq h(Z)\} = \int_{-\infty}^{x} h(z)g(z)\,\mathrm{d}z, \tag{3.69}$$

where $h(z)$ is the probability of success given z and $g(z)\,\mathrm{d}z$ is the probability that z is in $\mathrm{d}z$. We may write the joint probability as the product of a marginal probability for success and a conditional probability that $Z < x$:

$$P\{Z < x \text{ and success}\} = P\{\text{success}\}P\{Z < x|\text{success}\}.$$

But, $P\{Z < \infty\} = 1$ so that

$$P\{\text{success}\} = \int_{-\infty}^{\infty} h(z)g(z)\,\mathrm{d}z.$$

The rejection technique yields a value for X only when a success occurs, that is,

$$P\{Z < x|\text{success}\} = \text{distribution of } Z\text{'s coming from a rejection algorithm}$$
$$= \frac{\int_{-\infty}^{x} h(z)g(z)\,\mathrm{d}z}{\int_{-\infty}^{\infty} h(z)g(z)\,\mathrm{d}z}; \tag{3.70}$$

therefore, the probability distribution that results from the rejection technique is

$$\frac{h(z)g(z)}{\int_{-\infty}^{\infty} h(t)g(t)\,\mathrm{d}t}.$$

However, we want to sample X from $f(x)$. If we choose

$$h(z) = \frac{f(z)/g(z)}{B_h}, \tag{3.71}$$

where B_h is an upper bound for $\frac{f(z)}{g(z)}$ and $h(z) \leq 1$; X will be sampled from

$$\frac{h(z)g(z)}{\int_{-\infty}^{\infty} h(t)g(t)\,\mathrm{d}t} = \frac{f(x)}{B_h \int_{-\infty}^{\infty} h(t)g(t)\,\mathrm{d}t} = f(x). \tag{3.72}$$

The a priori probability of a success is called the efficiency, ϵ, and is given by

$$P\{\text{success}\} = \epsilon = \int_{-\infty}^{\infty} h(z)g(z)\,\mathrm{d}z. \tag{3.73}$$

The efficiency for the choice of $h(z)$ in Equation 3.71 becomes

$$\epsilon = \frac{1}{B_h} \int_{-\infty}^{\infty} \left[\frac{f(z)}{g(z)}\right] g(z)\,\mathrm{d}z = \frac{1}{B_h} \tag{3.74}$$

since $\int_{-\infty}^{\infty} f(z)\,\mathrm{d}z = 1$. B_h should be the least upper bound for $\frac{f(z)}{g(z)}$ to maximize the efficiency.

The expected number of trials up to and including a success per accepted random variable is (cf. Section 2.2.2)

$$\sum_{k=0}^{\infty} (k+1)(1-\epsilon)^k \epsilon = \frac{1}{\epsilon}. \tag{3.75}$$

A better measure of the usefulness of a rejection technique is the expected number of trials multiplied by the computer time per trial.

Let us consider again the example in Equation 3.68

$$f(x) = \frac{4}{\pi} \frac{1}{1+x^2},$$

and set $B_h = \frac{4}{\pi}$. The efficiency of the rejection technique is $\epsilon = \frac{\pi}{4}$ and the expected number of trials up to and including the first success is $\frac{4}{\pi}$. The proposed algorithm for sampling an X is

1. $Z = \xi_1$;
2. if $\xi_2 > \frac{1}{(1+Z^2)}$, then repeat from 1; otherwise accept $X = Z$.

The time per accepted X using this algorithm on a microprocessor was found to be 0.5×10^{-6} seconds. An alternative, inversion method for sampling $f(x)$ discussed previously is

$$X = \tan \frac{\pi}{4} \xi.$$

Using the same compiler, pseudorandom number generator and microprocessor, the time for choosing an X from the latter method was 0.4×10^{-6} seconds. Even though the rejection technique requires sampling two uniform random numbers as well as the possibility of multiple iterations of the loop, the time per accepted value is comparable to the inversion method.

3.5.1
Sampling a Singular pdf Using Rejection

Consider the singular probability distribution function

$$f(x) = \frac{2}{\pi(1-x^2)^{\frac{1}{2}}}, \quad 0 < x < 1; \tag{3.76}$$

this function is unbounded and the straightforward rejection technique introduced above is not appropriate here. Instead, write

$$f(x) = \frac{2}{\pi}\frac{1}{(1+x)^{\frac{1}{2}}(1-x)^{\frac{1}{2}}}$$

and let

$$g(z) = \frac{1}{2(1-z)^{\frac{1}{2}}}; \tag{3.77}$$

then $f(z)/g(z)$ becomes

$$\begin{aligned}\frac{f(z)}{g(z)} &= \frac{2}{\pi}\frac{1}{(1+z)^{\frac{1}{2}}(1-z)^{\frac{1}{2}}} \times 2(1-z)^{\frac{1}{2}} \\ &= \frac{4}{\pi}\frac{1}{(1+z)^{\frac{1}{2}}} \leq \frac{4}{\pi}.\end{aligned} \tag{3.78}$$

An appropriate choice for $h(z)$ is

$$h(z) = \frac{f(z)/g(z)}{B_h} = \frac{1}{(1+z)^{\frac{1}{2}}},$$

with $B_h = \frac{4}{\pi}$. An algorithm for selecting an X is

1. sample Z from $\frac{1}{2}(1-z)^{\frac{1}{2}}$ (i.e. $Z = 1 - \xi_1^2$);
2. if $\xi_2 \leq \frac{1}{(1+Z)^{\frac{1}{2}}}$, set $X = Z$; else reject and repeat from 1.

Step 2 may be written more efficiently as $\xi_2^2(1+Z) \leq 1$ to avoid a square root and a division.

3.5.2
Sampling the Sine and Cosine of an Angle

Rejection techniques have been used extensively in Monte Carlo calculations. A particularly famous algorithm is due to von Neumann [4] for sampling the sine and cosine of an angle uniform on $(0, 2\pi)$. If we are interested in the rotation of objects in three-dimensional space, the angle of rotation may be sampled uniformly, but the sine and cosine of the angle must be calculated for the rotation matrix. The straightforward method would set

$$\Phi = 2\pi\xi$$

and then calculate $\cos\Phi$ and $\sin\Phi$. It would be more efficient to have another method of sampling Φ that gives the sine and cosine directly. Consider the unit quarter circle inscribed inside the unit square as in Figure 3.13. The direction inside the quarter circle is uniformly distributed

$$f(\phi)\,\mathrm{d}\phi = \frac{2}{\pi}\,\mathrm{d}\phi.$$

The probability of finding an angle in $\mathrm{d}\phi$ is proportional to $\mathrm{d}\phi$. Values of X and Y are chosen uniformly on $(0, 1)$:

1. $X = \xi_1$ and $Y = \xi_2$;
2. if $(X^2 + Y^2 > 1)$, reject and repeat from 1;
3. otherwise set $\Phi = \tan^{-1} Y/X$.

The cosine and the sine in terms of X and Y are

$$\cos\Phi = \frac{X}{(X^2+Y^2)^{\frac{1}{2}}} = \frac{\xi_1}{(\xi_1^2+\xi_2^2)^{\frac{1}{2}}}, \tag{3.79a}$$

$$\sin\phi = \frac{Y}{(X^2+Y^2)^{\frac{1}{2}}} = \frac{\xi_2}{(\xi_1^2+\xi_2^2)^{\frac{1}{2}}}. \tag{3.79b}$$

If ϕ is uniformly distributed on $\left(0, \frac{\pi}{2}\right)$, then 2ϕ is uniformly distributed on $(0, \pi)$ and a square root may be avoided by calculating

$$\cos 2\Phi = \cos^2\Phi - \sin^2\Phi = \frac{X^2 - Y^2}{X^2 + Y^2}, \tag{3.80a}$$

$$\sin 2\Phi = 2\sin\Phi\cos\Phi = \frac{2XY}{X^2+Y^2}. \tag{3.80b}$$

In many calculations (e.g. in selecting direction in three dimensions), however, the $\sin\phi$ and $\cos\phi$ are used in association with a square root. In these circumstances, there is no disadvantage in using Equation 3.79 since the square roots can be combined.

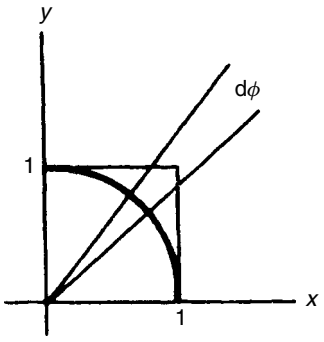


Figure 3.13 Sampling for $\sin\phi$ and $\cos\phi$.

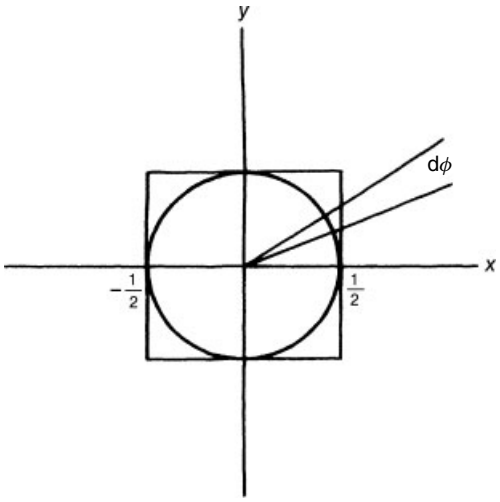


Figure 3.14 Sampling Φ uniformly over the unit circle.

If the angle ϕ is to be defined on $(0, 2\pi)$, then Equation 3.80b becomes

$$\sin 2\Phi = \pm\frac{2XY}{X^2 + Y^2}, \tag{3.80c}$$

where a third random number, ξ_3, is used to choose the sign. An alternative method is to select Φ uniformly over the circle whose diameter is 1 as shown in Figure 3.14, and set $X = \xi_1 - \frac{1}{2}$ and $Y = \xi_2 - \frac{1}{2}$. The values of X and Y are accepted only if $X^2 + Y^2 < \frac{1}{4}$, and Equations 3.79 and 3.80a follow as before.

3.5.3
Kahn's Rejection Technique for a Gaussian

Another rejection technique, introduced by Kahn [1], is used to sample a Gaussian. The function

$$\phi'(x) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}x^2\right], \quad 0 < x < \infty$$

cannot be bounded within a rectangle since its argument has infinite range. To sample $\phi'(x)$, we must sample from a function defined on the same range. Suppose x has the pdf $\alpha e^{-\alpha x}$, $0 < x < \infty$, and y has the pdf e^{-y}, $0 < y < \infty$; random variables X and Y are chosen by

$$X = -\frac{1}{\alpha}\log \xi_1,$$
$$Y = -\log \xi_2.$$

The value for X is kept if

$$Y > \tfrac{1}{2}(X - \alpha)^2;$$

otherwise new values for X and Y are selected. The probability that X is accepted (success) is

$$\epsilon = \int_{\left(\frac{1}{2}\right)(x-\alpha)^2}^{\infty} \mathrm{e}^{-y}\,\mathrm{d}y \tag{3.81}$$

and the joint probability that $X < x$ and success becomes

$$\begin{aligned} P\{X < x \text{ and success}\} &= \int_0^x \alpha \mathrm{e}^{-\alpha t} \int_{\left(\frac{1}{2}\right)(t-\alpha)^2}^{\infty} \mathrm{e}^{-u}\,\mathrm{d}u\,\mathrm{d}t \\ &= \int_0^x \alpha \mathrm{e}^{-\alpha t} \mathrm{e}^{-\left(\frac{1}{2}\right)(t-\alpha)^2}\,\mathrm{d}t \\ &= \alpha \mathrm{e}^{-\left(\frac{1}{2}\right)\alpha^2} \int_0^x \mathrm{e}^{-\left(\frac{1}{2}\right)t^2}\,\mathrm{d}t. \end{aligned} \tag{3.82}$$

Therefore, the probability distribution function for an accepted X is proportional to a Gaussian:

$$f(x) = \mathrm{e}^{-\left(\frac{1}{2}\right)x^2}.$$

A sign to be associated with X would be chosen randomly so that the range is $(-\infty, \infty)$. The proposed algorithm is correct for any positive α, but the efficiency will vary with α:

$$\begin{aligned} \epsilon &= \alpha \mathrm{e}^{-\left(\frac{1}{2}\right)\alpha^2} \int_0^{\infty} \mathrm{e}^{-\left(\frac{1}{2}\right)x^2}\,\mathrm{d}x \\ &= \sqrt{\frac{\pi}{2}} \alpha \mathrm{e}^{-\left(\frac{1}{2}\right)\alpha^2}. \end{aligned}$$

The maximum efficiency occurs when $\alpha = 1$. The Kahn rejection technique compares favorably with the Box–Muller method (Equation 3.38) for sampling a Gaussian.

3.5.4
Marsaglia *et al.* Method for Sampling a Gaussian

Marsaglia *et al.* [5] have developed composition methods that are particularly fast and efficient using random access to store fairly large lookup tables. A pdf is written

$$f(x) = \sum_{i=1}^{n} b_i g_i(x).$$

The $g_i(x)$ that is sampled the most frequently is chosen to involve a fast table lookup. In the case of the Gaussian distribution,

$$f(x) = 0.9578 g_1(x) + 0.0395 g_2(x) + 0.0027 g_3(x).$$

$g_1(x)$ and $g_2(x)$ are discrete pdf's that are stored in a table. $g_2(x)$ also involves a rejection. $g_1(x)$ is sampled rapidly and provides X 95% of the time. $g_3(x)$ is used to sample the tail of the Gaussian and involves a technique similar to that proposed by Box–Muller. Though the rejection method is much slower than the table lookup, it will occur only 0.27% of the time. Thus, overall, Marsaglia's method will generate Gaussian variables much more efficiently than a straight rejection technique.

3.6 Multivariate Distributions

Except for the bivariate normal distribution, which was introduced as a technical device, our treatment of sampling has been devoted to random variables in one dimension. Multivariate distributions are also important since Monte Carlo is at its best in treating many-dimensional problems. One may use the ideas of marginal and conditional distributions (Equation 2.31 and the discussion that follows) to reduce multivariate to univariate sampling. As usual the point is most easily discussed by an illustration, a pdf of a random variable in $\boldsymbol{R}^3$, $\boldsymbol{x} = (x, y, z)$:

$$f(\boldsymbol{x}) = \frac{1}{8\pi} e^{-r}, \tag{3.83}$$

where $r = \sqrt{x^2 + y^2 + z^2}$. The volume element dV that is associated with $f(\boldsymbol{x})$ is $dx\, dy\, dz$. In polar coordinates, $dV = r^2\, dr\, \sin\theta\, d\theta\, d\phi$ and

$$f(\boldsymbol{x})\, dx\, dy\, dz = \frac{1}{8\pi} e^{-r} r^2\, dr sin\theta\, d\theta\, d\phi, \tag{3.84}$$

where the polar coordinates are defined as

$$\cos\theta = z/r, \quad \tan\phi = y/x.$$

Equation 3.84 can be written as the product of three pdf's,

$$f(\boldsymbol{x})\, dV = \frac{1}{2} r^2 e^{-r}\, dr \frac{sin\theta\, d\theta}{2} \frac{d\phi}{2\pi}, \tag{3.85}$$

and r, θ, and ϕ may be sampled independently. A random variable that will be distributed as $r^2 e^{-r}$ can be sampled[3] by

$$\begin{aligned} R &= -\sum_{i=1}^{3} \log \xi_i \\ &= -\log(\xi_1 \times \xi_2 \times \xi_3). \end{aligned}$$

The random variable Φ is distributed uniformly on $(0, 2\pi)$, so

$$\Phi = 2\pi\xi_5.$$

3) Note that generally the sum of n independent random variables each with pdf e^{-x} is distributed as $x^{n-1}e^{-x}/(n-1)!$

The probability distribution for θ can be rewritten as

$$\frac{\sin\theta\,\mathrm{d}\theta}{2} = -\frac{\mathrm{d}(\cos\theta)}{2}.$$

Since $\cos\theta$ is uniformly distributed on $(-1, 1)$, it can be sampled by

$$\cos\ \Theta = 2\xi_4 - 1. \tag{3.86}$$

An alternative derivation of Equation 3.86 is arrived at by setting $F(\theta)$ equal to a uniform random number:

$$\frac{1}{2}\int_0^\theta \sin\ \theta\,\mathrm{d}\theta = \frac{\cos\ \theta}{2} + \frac{1}{2} = \xi.$$

If ξ is replaced by $1 - \xi_4$, then the last equation reduces to Equation 3.86. In many applications, it will be X, Y, and Z that are required:

$$Z = R\ \cos\ \Theta,$$

$$X = R\ \sin\ \Theta\cos\ \Phi,$$

$$Y = R\ \sin\ \Theta\sin\ \Phi.$$

In this case, it will be more efficient to calculate $\cos\ \Phi$ and $\sin\ \Phi$ directly, as described in Section 3.5.2. Also, since $\sin\theta = (1 - \cos^2\ \theta)^{\frac{1}{2}}$, there will be no loss in efficiency by using the von Neumann rejection technique, which contains square roots (Equation 3.79).

Singular probability distribution functions are as easily sampled in many dimensions as in one dimension. Let $f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{V}$ be the singular pdf

$$\begin{aligned} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{V} &= \frac{1}{4\pi}\frac{1}{r^2}\,\mathrm{e}^{-r}\,\mathrm{d}\boldsymbol{V} \\ &= \frac{1}{4\pi}\frac{1}{r^2}\,\mathrm{e}^{-r}r^2\,\mathrm{d}r\,\mathrm{d}(\cos\ \theta)\,\mathrm{d}\phi \\ &= \mathrm{e}^{-r}\,\mathrm{d}r\frac{\mathrm{d}(\cos\theta)}{2}\frac{\mathrm{d}\phi}{2\pi}. \end{aligned}$$

The random variables $\cos\Theta$ and Φ are sampled as described above and R can be sampled by

$$R = -\log\xi.$$

3.6.1 Sampling a Brownian Bridge

In a number of interesting applications (e.g. [6]), it becomes necessary to sample a "Brownian bridge" or Brownian motion (see Section 5.2.4) "tied down," which may be defined as follows. For some integer M and real numbers τ and x_i, $0 \le i \le M$, let

$$B(x_0, x_1, \ldots, x_M, \tau) = \sqrt{2\pi M\tau}\, e^{(x_M - x_0)^2/(2M\tau)} \prod_{i=1}^{M} \frac{e^{-(x_{i-1}-x_i)^2/(2\tau)}}{\sqrt{2\pi\tau}} \tag{3.87}$$

and

$$\int \cdots \int B(x_0, x_1, \ldots, x_M, \tau)\, dx_1\, dx_2 \ldots dx_{M-1} = 1.$$

Suppose that x_0 and x_M are fixed and it is required to sample the variables $x_1, x_2, \ldots, x_{M-1}$. To accomplish this, we compute a marginal distribution for (say) x_j, $0 < j < M$, by integrating over $x_1, x_2, \ldots, x_{j-1}, x_{j+1}, \ldots, x_{M-1}$. The identity

$$\int \frac{e^{-(x-y)^2/(2\sigma_1^2)}}{\sqrt{2\pi\,\sigma_1^2}} \frac{e^{-(y-z)^2/(2\sigma_2^2)}}{\sqrt{2\pi\,\sigma_2^2}}\, dy = \frac{e^{-(x-z)^2/(2(\sigma_1^2+\sigma_2^2))}}{\sqrt{2\pi(\sigma_1^2+\sigma_2^2)}}$$

may be used recursively to find

$$\begin{aligned}
&\int \cdots \int B(x_0, x_1, \ldots, x_M, \tau)\, dx_1\, dx_2 \ldots dx_{j-1}\, dx_{j+1} \ldots dx_{M-1} \\
&\quad = \sqrt{2\pi M\tau}\, e^{(x_M - x_0)^2/(2M\tau)} \frac{e^{-(x_0-x_j)^2/(2j\tau)}}{\sqrt{2\pi j\tau}} \frac{e^{-(x_j-x_M)^2/(2(M-j)\tau)}}{\sqrt{2\pi(M-j)\tau}} \\
&\quad \equiv \frac{e^{-(x_j-\overline{x})^2/(2\sigma_j^2)}}{\sqrt{2\pi\,\sigma_j^2}},
\end{aligned} \tag{3.88}$$

where

$$\overline{x} = \frac{jx_M + (M-j)x_0}{M},$$
$$\sigma_j^2 = \frac{j(M-j)\tau}{M}.$$

Thus, the marginal distribution for x_j given x_0 and x_M is a Gaussian or normal distribution, Equation 3.88, with mean $\overline{x}$ and variance σ_j^2, and may be sampled in any of the ways discussed previously in Sections 3.1 and 3.5. Then given x_j and x_0, one may sample x_k, $0 < k < j$, using a Gaussian distribution with mean $(kx_j + (j-k)x_0)/j$ and variance $k(j-k)\tau/j$. Similarly, given x_j and x_M one may sample $x_\ell, j < \ell < M$, from a Gaussian distribution with mean $((\ell - j)x_M + (M-\ell)x_j)/(M-j)$ and variance $(\ell - j)(M-\ell)\tau/(M-j)$.

One technique that is often used is to let M be 2^n and use recursive bisection in which j is first set to $2(n-1)$ and the intervals are successively halved. As shown above, this is not necessary; one can equally well use $j = 1$, $k = 2$, etc.

The generalization to more dimensions follows a similar approach. The variable $\overline{x}$ becomes the mean of two vectors, and the x_j is sampled from the appropriate multivariate Gaussian distributions.

3.7 The M(RT)^2 Algorithm

The last sampling method we shall discuss is an advanced sampling technique first described in a paper by Metropolis *et al.* [7] [M(RT)^2].[4] The method is related to rejection techniques since it involves explicitly proposing a tentative value that may be rejected and because the normalization of the sampled function is irrelevant, we never need to know it.

The M(RT)^2 algorithm is very simple and powerful; it can be used to sample essentially any distribution function regardless of analytic complexity in any number of dimensions. Complementary disadvantages are that sampling is correct only asymptotically and that successive variables produced are correlated, often very strongly. This means that the evaluation of integrals normally produces positive correlations in the values of the integrand, with consequent increase in variance for a fixed number of steps as compared with independent samples. Also the method is not well suited to sampling distributions with parameters that change frequently.

The usual description of the M(RT)^2 method can be found in the papers by Valleau and Whittington [8] and Valleau and Torrie [9], Wood and Erpenbeck [10], and Allen and Tildesley [11]. Here we shall develop a somewhat more general description.

The method was motivated by an analogy with the behavior of systems in statistical mechanics that approach an equilibrium whose statistical properties are independent of the kinetics of the system.

By *system*, we mean here simply a point x in a space Ω (typically in $\boldsymbol{R}^M$) that may be thought of as a possible description of a physical problem. By *kinetics*, we mean a stochastic transition that governs the evolution of the system: a probability distribution function $K(X|Y)$ that ensures the evolution of a system known to be at Y will bring it near X next. K may be thought of as a model of the physical process by which a system changes or as a mathematical abstraction. In a Monte Carlo calculation, it plays the role of a sampling distribution.

As we shall discuss in detail, one condition for a system to evolve toward equilibrium and stay there is, quite simply, that the system be on the average as likely to move into a specific neighborhood of X from a neighborhood of Y as to move exactly in the reverse direction. If the probability distribution for observing the system near X in equilibrium is $f(X)$, then the kinetics must satisfy

$$K(X|Y)f(Y) = K(Y|X)f(X). \tag{3.89}$$

This relation is called *detailed balance* [12]. $K(X|Y)f(Y)$ is the probability of moving from Y to X expressed as the a priori chance of finding the system near Y (i.e. $f(Y)$) times the conditional probability $[K(X|Y)]$ that it will move to X from Y.

In treating a physical system, one usually assumes that $K(X|Y)$ is known, and one has the task of finding $f(X)$. The M(RT)^2 algorithm (as in much of Monte

4) In the literature, it is often referred to as the Metropolis algorithm.

Carlo) reverses this: one has the task of finding a convenient and correct kinetics that will equilibrate the system so that the given $f(X)$ turns out to be the chance of observing the system near X.

This turns out to be extremely easy given the elegant device suggested by M(RT)^2. Transitions are *proposed* from, say, Y to X' using essentially *any* distribution $T(X'|Y)$. Then on comparing $f(X')$ with $f(Y)$ and taking into account T as well, the system is either moved to X' (move "accepted") or returned to Y (move "rejected"). Acceptance of the move occurs with probability $A(X'|Y)$, which must be calculated so as to satisfy detailed balance.

We then have

$$K(X|Y) = A(X|Y)T(X|Y). \tag{3.90}$$

Detailed balance requires

$$A(X|Y)T(X|Y)f(Y) = A(Y|X)T(Y|X)f(X). \tag{3.91}$$

We expect that the ratio

$$\frac{T(Y|X)\,f(X)}{T(X|Y)\,f(Y)}$$

will play a significant role in determining A.

Given a pdf $f(X)$, where X is a many-dimensional vector, the M(RT)^2 technique establishes a random walk whose steps are designed so that when repeated again and again, the asymptotic distribution of X's is $f(X)$. Suppose that $X_1, X_2, X_3, \ldots, X_n$ are the steps in a random walk. Each of the X's is a random variable and has an associated probability $\phi_1(X), \phi_2(X), \phi_3(X), \ldots, \phi_n(X)$, where $\phi_1(X)$ can be any distribution for X. The $\phi_n(X)$ have the property that asymptotically

$$\lim_{n\to\infty} \phi_n(X) = f(X).$$

At each step, in the random walk, there is a transition distribution $T(X|Y)$, that is, the probability distribution function for a trial move to X from Y. The $T(X|Y)$ is normalized such that

$$\int T(X|Y)\,\mathrm{d}X = 1$$

for all values of Y. A quantity $q(X|Y)$ is defined as

$$q(X|Y) = \frac{T(Y|X)f(X)}{T(X|Y)f(Y)} \geq 0, \tag{3.92}$$

where we explicitly assume that it is possible to move from X to Y if one can move from Y to X and vice versa. From $q(X|Y)$, the probability of accepting a move can be calculated; one frequently used possibility is

$$A(X|Y) = \min(1, q(X|Y)). \tag{3.93}$$

The algorithm can now be described concretely. At step n of the random walk, the value of X is X_n; a possible next value for X, X'_{n+1}, is sampled from $T(X'_{n+1}|X_n)$, and the probability of accepting X'_{n+1} is computed. If $q(X'_{n+1}|X_n) > 1$ then $A(X'_{n+1}|X_n) = 1$; if $q(X'_{n+1}|X_n) < 1$, then $A(X'_{n+1}|X_n) = q(X'_{n+1}|X_n)$, where

$$q(X'_{n+1}|X_n) = \frac{T(X_n|X'_{n+1})f(X'_{n+1})}{T(X'_{n+1}|X_n)f(X_n)}.$$

With probability $A(X'_{n+1}|X_n)$, we set $X_{n+1} = X'_{n+1}$; Otherwise, we set $X_{n+1} = X_n$. That is, if $A(X'_{n+1}|X_n) > \xi$, then $X_{n+1} = X'_{n+1}$; otherwise, $X_{n+l} = X_n$. For $q(X'_{n+1}|X_n) > 1$, X_{n+1} will always equal X'_{n+1}. This procedure contains an element of rejection; however, if an X'_{n+1} is not accepted, we use the previous value rather than sample a new value.

As the random walk proceeds, a recursive relationship develops between succeeding $\phi_n(X)$'s. Let $\phi_n(X)$ be the distribution of values of X_n; what is the distribution ϕ_{n+1} for the values of X_{n+1}? There are two contributions to the distribution of the X_{n+1}: the probability of entering into the vicinity $\mathrm{d}X$ of X when we successfully move from X_n and the probability that once we are at X, we will stay at X. If we start out at some value Y contained in $\mathrm{d}Y$, the probability of moving from the neighborhood of Y to the neighborhood of X is $T(X|Y)\phi_n(Y)\,\mathrm{d}Y$. The probability of successfully moving from Y to X is $A(X|Y)T(X|Y)\phi_n(Y)\,\mathrm{d}Y$, so the net probability of successfully moving from any point Y to a neighborhood of X becomes

$$\int A(X|Y)T(X|Y)\phi_n(Y)\,\mathrm{d}Y. \tag{3.94}$$

In a similar manner, the net probability that a move away from X is not accepted is

$$\int (1 - A(Y|X))T(Y|X)\,\mathrm{d}Y, \tag{3.95}$$

where $T(Y|X)$ is the probability of moving from X to Y and $[1 - A(Y|X)]$ is the probability that the move was not accepted. Upon multiplying Equation 3.95 by $\phi_n(X)$, the probability that we were at X, the relationship for $\phi_{n+1}(X)$ becomes

$$\phi_{n+1}(X) = \int A(X|Y)T(X|Y)\phi_n(Y)\,\mathrm{d}Y + \phi_n(X)\int [1 - A(Y|X)]T(Y|X)\,\mathrm{d}Y. \tag{3.96}$$

The random walk generates a recursion relationship for the distribution functions.

Earlier, we asserted that the asymptotic distribution sampled in the random walk would be $f(X)$. According to a theorem in Feller [13], if a random walk defines a system that is ergodic, then an asymptotic pdf exists and is unique if

$$\phi_n(X) = f(X) \;\Rightarrow\; \phi_{n+1}(X) = f(X), \tag{3.97}$$

that is, if $f(X)$ is a stationary point of the recursion. Systems defined by random walks can be partitioned into several categories. If, in a random walk, the probability of

returning to a neighborhood about X is 0, then the system is called a *null system* and the expected recurrence time is infinite. An example would be a one-dimensional system where X_{n+1} is constrained to be greater than X_n. A system where the random walk will return to the neighborhood of X every T steps is called *periodic*. An ergodic system is one in which the random walk may return to the neighborhood of X, but does not do so periodically; it is neither null nor periodic.

The system generated by the M(RT)^2 sampling method is ergodic, but the proof will be omitted [14]. The system obeys detailed balance, which guarantees that, if we can move from X to Y, we can move from Y to X and the expected number of moves is the same in each direction when the asymptotic behavior is reached:

$$A(X|Y)T(X|Y)f(Y) = A(Y|X)T(Y|X)f(X). \tag{3.98}$$

The left-hand side is the net number of moves from Y to X and the right-hand side is the net number of moves from X to Y. Equation 3.98 is easily proved by using $q(X|Y)q(Y|X) = 1$, which follows from the definition of $q(X|Y)$. Suppose that $q(X|Y) > 1$; then $A(X|Y) = 1$. $A(Y|X) = q(Y|X)$ since $q(Y|X) < 1$. Substituting these into Equation 3.98, we derive

$$\begin{aligned} T(X|Y)f(Y) &= q(Y|X)T(Y|X)f(X) \\ &= \frac{T(X|Y)f(Y)}{T(Y|X)f(X)}T(Y|X)f(X). \end{aligned}$$

The same answer would have resulted if we had chosen $q(Y|X) > 1$, so the algorithm developed in Equations 3.92 and 3.93 satisfies detailed balance.

If we set $\phi_n(X) = f(X)$ in Equation 3.96, the resulting equation is

$$\phi_{n+1}(X) = \int A(X|Y)T(X|Y)f(Y)\,\mathrm{d}Y + \int [1 - A(Y|X)]T(Y|X)f(X)\,\mathrm{d}Y.$$

The first integral cancels the negative portion of the second integral by detailed balance, and we are left with

$$\begin{aligned} \phi_{n+1}(X) &= \int T(Y|X)f(X)\,\mathrm{d}Y \\ &= f(X) \end{aligned}$$

since $\int T(Y|X)\,\mathrm{d}Y = 1$. Therefore, $f(X)$ is guaranteed to be the asymptotic distribution of the random walk.

The form for the probability of accepting a move is not limited to that given in Equation 3.93. Another relation that has been used is

$$A'(X|Y) = \frac{q(X|Y)}{1 + q(X|Y)}$$

and

$$A'(Y|X) = \frac{q(Y|X)}{1 + q(Y|X)} = \frac{1}{q(X|Y) + 1}. \tag{3.99}$$

A random walk whose probability of accepting a move is governed by Equation 3.99 also exhibits detailed balance:

$$A'(X|Y)T(X|Y)f(Y) = A'(Y|X)T(Y|X)f(X).$$

Upon substituting Equation 3.99 for A' on both sides of the equation we find

$$\frac{q(X|Y)}{1+q(X|Y)}T(X|Y)f(Y) = \frac{1}{1+q(X|Y)}T(Y|X)f(X), \tag{3.100}$$

which reduces to

$$\frac{T(Y|X)f(X)}{T(X|Y)f(Y)}T(X|Y)f(Y) = T(Y|X)f(X).$$

Either form for $A(X|Y)$, Equation 3.93 or 3.99, may be used in the M(RT)^2 method. The former has been shown to give more rapid convergence in certain cases [8].

In much of the literature of statistical physics, when a Monte Carlo calculation is mentioned what is meant is an application of the method of Metropolis *et al.* The great utility of the M(RT)^2 method is that it enables us to sample very complicated many-dimensional probability distribution functions in a simple, straightforward way. Unfortunately, the method does have major drawbacks of which the user must be aware. We are guaranteed to sample $f(X)$, but only asymptotically; therefore, we must throw away L steps of the random walk until the steps are being sampled from $f(X)$. Furthermore, L is very difficult to estimate in advance. Normally, substantial trial and error is used to estimate an appropriate value. The number of steps discarded may be minimized by selecting a $\phi_1(X)$ that is as close an approximation to $f(X)$ as possible. In addition, by making $T(X|Y)$ approximate $f(X)$, rapid convergence and small correlation are obtained. Note that were it possible to sample $T(X|Y) = f(X)$ exactly, then (cf. Equations 3.92 and 3.93) all moves are accepted and the samples are independent. In that case, of course, one would not resort to the M(RT)^2 random walk, but it is clear that approximations to this limiting case may be fruitful.

In a Monte Carlo calculation, we are often trying to evaluate quantities of the form

$$G = \frac{\int g(X)f(X)\,\mathrm{d}X}{\int f(X)\,\mathrm{d}X}.$$

For example, if we are trying to simulate the equilibrium properties of a many-body system, G might be the energy or the *radial distribution function* (the probability that pairs of particles are found at varying separations). In practice, for each quantity of interest, a different number of steps in the random walk may have to be discarded since the asymptotic limit of the system is reached at varying rates. The averaging over the steps in the random walk begins only after the L steps have been thrown away, that is,

$$G = \frac{\int g(X)f(X)\,\mathrm{d}X}{f(X)\,\mathrm{d}X} = \sum_{n=L}^{L+N-1}\frac{g(X_n)}{N}.$$

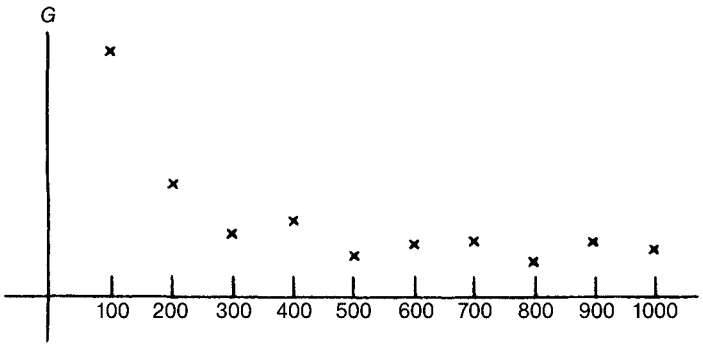


Figure 3.15 Behavior of $\langle G \rangle$ with length of the M(RT)^2 random walk.

The successive X's in the random walk are *not* independent and in most circumstances there is positive correlation. The variance of the calculated G will then be larger than if the steps were independent.

The number of steps to be discarded before averaging must be determined experimentally. One way is to average some property of the system, G, over (say) every 100 steps and observe the behavior of G with increasing walk length. An illustration of the behavior of G is shown in Figure 3.15. A decision is then made about where in the random walk the value of G has converged; further variation is just the normal wandering that occurs in a random walk. All contributions prior to this point are discarded, and an average for G is extracted from the remaining steps. Careless observation of the attainment of the asymptotic distribution in the M(RT)^2 method has led to some bad Monte Carlo calculation in the past.

The usage of the M(RT)^2 method can be illustrated by some trivial examples. Almost without exception in applications, the transition distribution $T(X|Y)$ is assumed to be constant over a domain in X. Consider the one-dimensional pdf shown in Figure 3.16, defined on $(0, 1)$. A possible algorithm is to sample an x uniformly in a domain centered on Y and define the transition probability as

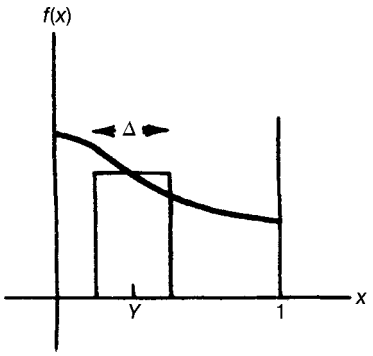


Figure 3.16 Monotonically decreasing pdf.

$$T(X|Y) = \begin{cases} \dfrac{1}{\Delta} & \text{if } |X - Y| < \dfrac{\Delta}{2} \\ 0 & \text{otherwise,} \end{cases}$$

where Δ is the width of the domain about Y. For this choice of $T(X|Y)$, $q(X|Y)$ becomes

$$q(X|Y) = \frac{T(Y|X)f(X)}{T(X|Y)f(Y)} = \frac{(1/\Delta)f(X)}{(1/\Delta)f(Y)} = \frac{f(X)}{f(Y)}. \tag{3.101}$$

(Note that this is the usual method for continuous distribution f.) In this example detailed balance requires that if an interval about Y contains X, the corresponding interval about X must contain Y. For values of Y not in the vicinity of the origin, moves to the left will always be accepted, whereas moves to the right will be accepted with probability $q(X|Y) = f(X)/f(Y)$. When Y is in the vicinity of the origin, all moves to the left tend to be rejected since $f(X) = 0$ when $x < 0$.

An equally good algorithm for the same example would be to choose

$$T(X|Y) = \begin{cases} 1, & X \in (0,1) \\ 0, & X \notin (0,1). \end{cases}$$

This corresponds to a uniform random sampling of X in $(0, 1)$.

The details of the M(RT)^2 method can fully be worked out for a one-dimensional example in which $f(X)$ is $2X$ on $(0, 1)$ and is 0 elsewhere. We can choose the transition distribution to be

$$T(X|Y) = \begin{cases} 1, & X \in (0,1) \\ 0, & \text{elsewhere} \end{cases}$$

and $q(X|Y)$ becomes, from Equation 3.92,

$$q(K|Y) = \begin{cases} \dfrac{T(Y|X)f(X)}{T(X|Y)f(Y)} = \dfrac{X}{Y}, & X \in (0,1) \\ 0, & \text{elsewhere.} \end{cases}$$

$q(X|Y) < 1$ implies that $f(X) < f(Y)$ and $X < Y$. This occurs for a move to the left, which will then be accepted with probability X/Y. When $q(X|Y) > 1$, $f(X) > f(Y)$ and a move to the right occurs. Such a move is always accepted in this example. The distribution of X's at the $(n+1)$th step will be, from Equation 3.96,

$$\phi_{n+1}(X) = \int_X^1 \frac{X}{Y}\phi_n(Y)\,\mathrm{d}Y + \int_0^X \phi_n(Y)\,\mathrm{d}Y + \phi_n(X)\int_0^X \left(1 - \frac{Y}{X}\right)\mathrm{d}Y. \tag{3.102}$$

The first integral corresponds to the contribution from $g(X|Y) < 1$; the second contains the contributions when $q(X|Y) > 1$ (for which the probability of accepting the move is 1); and the third is the contribution from rejected steps.

Normalization is preserved in Equation 3.102. That is, if $\phi_n(X)$ is normalized, $\phi_{n+1}(X)$ will be too. If at some value of n, ϕ_n is linear and homogeneous, $\phi_n(X) = cX$, then $\phi_{n+1}(X) = cX$. This is true because Equation 3.102 is homogeneous and because putting $\phi_n(X) = 2X$ must and does generate $\phi_{n+1}(X) = 2X$.

Let us assume that at the nth step the distribution of X's is

$$\phi_n(X) = a_n X + c_n X^{n+2} \tag{3.103}$$

and

$$\phi_0(X) = 3X^2.$$

Equation 3.103 is substituted into Equation 3.102; the linear term $a_n X$ will carry through to give a contribution of $a_n X$ to $\phi_{n+1}(X)$. Applying the right-hand side of Equation 3.102 to $c_n X^{n+2}$, we get

$$c_n X \int_X^1 \frac{Y^{n+2}}{Y} \mathrm{d}Y + c_n \int_0^X Y^{n+2} \mathrm{d}Y + c_n X^{n+2} \int_0^X \left(1 - \frac{Y}{X}\right) \mathrm{d}Y$$
$$= c_n \frac{X}{n+2}(1 - X^{n+2}) + \frac{c_n}{n+3} X^{n+3} + \frac{c_n}{2} X^{n+3},$$

which contains terms of both X and X^{n+3}. The form of $\phi_{n+1}(X)$ becomes

$$\phi_{n+1}(X) = \left(a_n + \frac{c_n}{n+2}\right) X + c_n \left[\frac{1}{2} - \frac{1}{(n+2)(n+3)}\right] X^{n+3}, \tag{3.104}$$

so asymptotically c_n will decrease as 2^{-n}, and we can rewrite $\phi_{n+1}(X)$:

$$\phi_{n+1}(X) \cong a_{n+1} X + \frac{c}{2^n} X^{n+3}.$$

The distributions of X exhibit explicit convergence; as n increases, the second term, $\left(\frac{c}{2^n}\right) X^{n+3}$, will contribute only values of X near 1 (see Figure 3.17). The normalization of the $\phi_n(X)$ gives the form of a_{n+1} as

$$a_{n+1} \cong 2 - \frac{c}{(n+4)2^n},$$

which asymptotically approaches 2.

We have set $\phi_0(X) = 3X^2$, so $a_0 = 0$ and $c_0 = 3$. For $n + 1 = 1$, Equation 3.104 yields

$$\phi_1(X) = \tfrac{3}{2} X + X^3$$

or that $a_1 = \frac{3}{2}$ and $c_1 = 1$. Another iteration of Equation 3.104 gives

$$\phi_2(X) = \tfrac{11}{6} X + \tfrac{5}{12} X^4,$$

where $a_2 = \frac{11}{6}$ and $c_2 = \frac{5}{12}$; with only two steps a_n is easily seen to be approaching 2 and c_n is decreasing as approximately 2^{-n}.

The fact that at the nth stage $\phi_n(X)$ differs from $a_n X$ by a function like X^{n+2} shows that the error in integrating $\int \phi_n(X) g(X)\, \mathrm{d}X / \int \phi_n \mathrm{d}X$ instead of $\int 2X g(X)\, \mathrm{d}X$ will depend on $g(X)$. This is a special case of the remark made earlier that the number of steps to be discarded may depend on the properties of a system being computed.

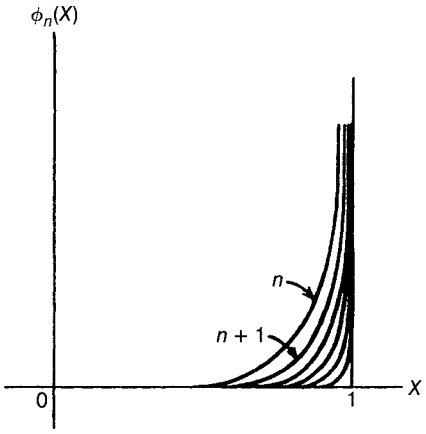


Figure 3.17 Behavior of $\phi_n(X)$ as n increases.

3.8 Application of M(RT)^2

As we have seen, when a pdf $f(x)$ must be sampled, M(RT)^2 gives a prescription for defining a random walk $X_0, X_1, \ldots$ for which the asymptotic distribution is guaranteed to be $f(X)$. These points X_i may be used to evaluate some integral by setting

$$\int g(X)f(X)\,dX \cong \frac{1}{M}\sum_{i=1}^{M} g(X_i).$$

Because $f(X)$ is sampled only asymptotically, the estimate of the integral is biased by an amount that can be made smaller by discarding more and more X_i at the beginning of the walk and by extending the walk to larger M. As we have indicated, the question of how many must be discarded can be answered only in the context of a specific problem. Nevertheless, it is necessary to give careful attention to this problem. It is this difficulty that makes M(RT)^2 unsuitable for applications in which only a few variables are sampled from a specific $f(X)$ with fixed parameters.

In the most usual applications, $T(X|Y)$ is taken to be uniform over a small domain (e.g. a square or cube of side s) in the space of X or in a subspace thereof. Let us consider a highly simplified model of atoms moving on the surface of something. Imagine a two-dimensional square box of side L that contains a large number ($10^2 - 10^4$) of disks (Figure 3.18). Each disk is located by the coordinates of its center and has an effective diameter a. If there are M disks, then we have $2M$ position coordinates, and a configuration of the system can be indicated by the vector

$$\mathbf{X} = (x_1, y_1, x_2, y_2, \ldots, x_m, y_m).$$

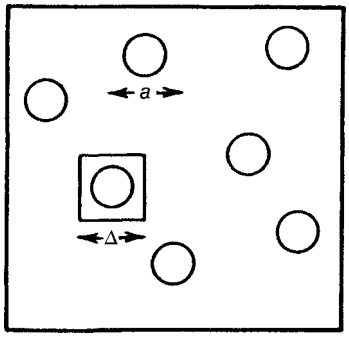


Figure 3.18 Hard disks in a box.

The pdf describing the system, $f(\boldsymbol{X})$, is a constant except when $x_k < 0$, $x_k > L$, or $(x_l - x_k)^2 + (y_l - y_k)^2 < a^2$ for any l and k. If any one of these conditions happens, $f(\boldsymbol{X}) = 0$. These restrictions prevent the disks from moving outside the box and from overlapping each other.

Given the two-dimensional system detailed above, what is the probability that two disks will be a distance r apart? We can answer this problem by using the M(RT)^2 method to generate many configurations, $\boldsymbol{X}$, and measure the frequency of occurrence of r. The problem would be difficult to analyze by any method other than M(RT)^2. A scheme for analyzing the problem in this way is to start with the disks on a lattice in the box so as to guarantee no overlap at the start. A disk is chosen randomly to be moved; the transition probability for moving from one configuration to another (the configurations differ by moving one disk) is

$$T(\boldsymbol{X}|\boldsymbol{Y}) = \sum_l f_l t(x_l, y_l | x_l', y_l'),$$

where

$$f_l = 1/M$$

and $t(x_l, y_l | x_l', y_l')$ is the transition distribution for moving uniformly in the little square. It is simply a constant, $1/\Delta^2$ where Δ is the side of the little square as in Figure 3.18. Thus, T is a constant and the ratio $\frac{T(\boldsymbol{Y}|\boldsymbol{X})}{T(\boldsymbol{X}|\boldsymbol{Y})}$ that appears in the acceptance probability is exactly 1. Once x_l and y_l have been calculated, the ratio $\frac{f(\boldsymbol{X})}{f(\boldsymbol{Y})}$ is evaluated. If the step has moved a disk outside the box or some disks are overlapping, then $f(\boldsymbol{X}) = 0$ and the move is rejected; otherwise, $\frac{f(\boldsymbol{X})}{f(\boldsymbol{Y})} = 1$ and the move is accepted. The process is repeated many times to generate many different configurations, and a frequency function for r is tabulated. The moves that occur do not describe physical motion of the disks since the "kinetics" introduced is completely artificial.

Some care must be exerted in the selection of the size of the little box surrounding a disk. In the limit that the individual box is the size of the whole domain (the big box), it will be unlikely to find an empty space in which to move a disk. Almost

all the moves will be rejected, so the random walk will be composed of the same configurations repeated many times. In this case, the sequential correlation from step to step is very close to one and the random walk provides very little new information at each step.

At the other extreme is a box too small. The move of the disk is always accepted, but the configuration changes very slowly. Again, there is high sequential correlation with little new information emerging as the particles are moved.

The "lore" for using the $M(RT)^2$ method recommends that the average acceptance probability should be approximately 50% to avoid both extremes described above. That is, the box size should be chosen such that 50% of the moves within it are accepted. A criterion for choosing the box size that has better justification but is harder to apply is to make moves within a box so that the variance in the desired result is minimized for given computing time. In this case, the variance is minimized by reducing the sequential correlation between steps. Sequential correlation decreases as the mean-square displacement increases. The mean-square displacement in one step is proportional to $p_A \Delta^2$. A simple usable criterion is to maximize this quantity where p_A is the average probability of acceptance. An acceptable value for Δ can be established by several trial runs in which Δ is changed and the variation in $\langle r^2 \rangle$ and p_A observed. The value of Δ that produces the maximum $\langle r^2 \rangle$ is then used in the actual calculation. This criterion has proved useful in practical cases. More generally, one should take account of the computer time used in the computation of $f(\boldsymbol{X})$.

3.9 Testing Sampling Methods

It is important to test that an algorithm indeed samples $f(x)$. Several methods to check the algorithm can be used. For few-dimensional distributions one may generate random variables and sort into bins within the range of the random variable. A frequency function is yielded by this method, and elementary statistical tests may be applied to it, for example, the number of times the observed frequency function is higher or lower than the expected value. A chi-squared test is appropriate. A third way of checking an algorithm is to use the algorithm to evaluate an elementary integral whose value is known, $\int g(x) f(x)\, dx$, and decide whether the value agrees within statistics with the correct value. Moments, in which $g_n = x^n$, are especially useful.

Consider the algorithm proposed by Wiener to sample two independent Gaussian random variables given in Equation 3.38. A subroutine is easily written to generate the random variables; we test this code by sampling from it many times and binning the result. After 5000 random samples, our frequency function for $\phi(x|0,1)$ appears as the bar graph[5] shown in Figure 3.19. The solid line represents the analytic values of Equation 3.36. A combination of such tests along

5) As with random sampling experiment, the details of the structure of this bar graph depend on the sequence of pseudorandom numbers used. A different sequence will give a different graph.

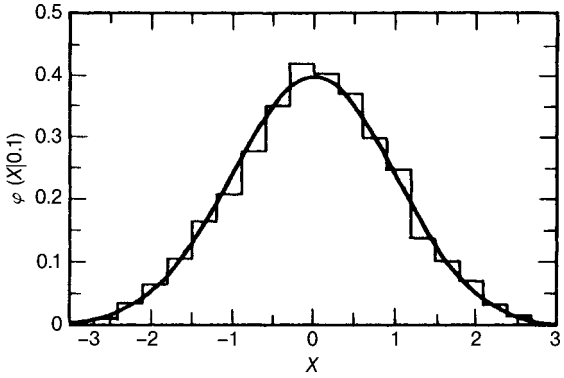


Figure 3.19 Frequency function after 1000 random samples of $\phi(x|0,1\}$.

with analysis of the hypothesis that the population is drawn from $f(x)$ is often warranted.

Such tests, if carefully carried out, constitute useful confirmations of the quality of the pseudorandom number sequences as well as of the sampling method under study.

The combination of logical complexity and statistical fluctuation means that Monte Carlo programs may require care in testing. Proper modular design of such programs is essential, and sampling routines constitute appropriate modules. The sampling routines should be thoroughly tested with specially designed "drivers," which evaluate the performance of the routines over a range of expected parameters. The final Monte Carlo code should be assembled from well-tested modules. Completion and analysis of a significant computation is not the ideal stage at which to uncover a "bug" in a sampling routine.

References

1 Kahn, H. (**1954**) Applications of Monte Carlo. AECU-3259, National Technical Information Service, U.S. Dept. of Commerce, Springfield, VA.

2 Everett, C.J. and Cashwell, E.D. (**1983**) A Third Monte Carlo Sampler. Los Alamos Technical Report LA-9721-MS, National Technical Information Service, U.S. Dept. of Commerce, Springfield, VA.

3 Box, G.E.P. and Muller, M.E. (**1958**) A note on the generation of random normal deviates. *Annals of Mathematical Statistics*, **29**, 610.

4 von Neumann, J. (**1951**) Various techniques used in connection with random digits. National Bureau of Standards. *Applied Mathematics Series*, **12**, 36.

5 Marsaglia, G., MacLaren, M.D. and Bray, T.A. (**1964**) A fast procedure for generation random variables. *Communications of the ACM*, **7**, 4.

6 Caflisch, R.E., Morokoff, W. and Owen, A. (**1997**) Valuation of mortgage-backed securities using brownian bridges to reduce effective dimension. *The Journal of Computational Finance*, **1**, 27.

7 Metropolis, N., Rosenbluth, A.W., Rosenbluth, M.N. *et al.* (**1953**)

Equations of state calculations by fast computing machines. *Journal of Chemical Physics*, **21**, 1087.

8 Valleau, J.P. and Whittington, S.G. (**1976**) A Guide to Monte Carlo for statistical mechanics: 1. Highways, in *Statistical Mechanics, Part A: Equilibrium Techniques, Modern Theoretical Chemistry Series*, Vol. 5, Chapter 4 (ed B. Berne), Plenum, New York.

9 Valleau, J.P. and Torrie, G.M. (**1976**) A guide to Monte Carlo for statistical mechanics: 2. Byways, in *Statistical Mechanics, Part A: Equilibrium Techniques, Modern Theoretical Chemistry Series*, Vol. 5, Chapter 5 (ed B. Berne), Plenum, New York.

10 Wood, W.W. and Erpenbeck, J.J. (**1976**) Molecular dynamics and Monte Carlo calculations in statistical mechanics. *Annual Review of Physical Chemistry*, **27**, 319.

11 Allen, M.P. and Tildesley, D.J. (**1993**) *Computer Simulation of Liquids*, Oxford University Press, Oxford.

12 Wood, W.W. (**1968**) Monte Carlo studies of simple liquid models, in *The Physics of Simple Liquids*, Chapter 5, Section 1 (eds H.N.V. Temperley, J.S. Rowlinson and G.S. Rushbrooke), North-Holland, Amsterdam.

13 Feller, W. (**1950**) *An Introduction to Probability Theory and Its Applications*, Vol. 1, John Wiley & Sons, Ltd, New York, p. 324.

14 Wood, W.W. and Parker, F.R. (**1957**) Monte Carlo equation of state of molecules interacting with the Lennard-Jones potential. I. Supercritical isotherm at about twice the critical temperature. *Journal of Chemical Physics*, **27**, 720.

Further Reading

Everett, C.J. and Cashwell, E.D. (**1983**) A Third Monte Carlo Sampler. Los Alamos Technical Report LA-9721-MS, National Technical Information Service, U.S. Dept. of Commerce, Springfield, VA.

Kahn, H. (**1954**) Applications of Monte Carlo. AECU-3259, National Technical Information Service, U.S. Dept. of Commerce, Springfield, VA.

Rubinstein, R.Y. (**1981**) *Simulation and the Monte Carlo Method*, John Wiley & Sons, Ltd, New York. Chapter 3 and references therein.

4
Monte Carlo Evaluation of Finite-Dimensional Integrals

In this chapter, we explore the ideas that underlie Monte Carlo quadrature somewhat more systematically. If an integral having the form

$$G = \int_{\Omega_0} g(x) f(x)\, \mathrm{d}x, \tag{4.1}$$

where

$$f(x) \geq 0, \quad \int_{\Omega_0} f(x)\, \mathrm{d}x = 1, \tag{4.2}$$

must be evaluated, then the following *game of chance* may be used to make numerical estimates. We draw a set of variables $X_1, X_2, \ldots, X_N$ from $f(x)$ (i.e. we "sample" the probability distribution function $f(x)$ in the sense defined in Chapter 3) and form the arithmetic mean

$$G_N = \frac{1}{N} \sum_i g(X_i). \tag{4.3}$$

The quantity G_N is an estimator for G and the fundamental theorem of Monte Carlo guarantees that

$$\langle G_N \rangle = G$$

if the integral (Equation 4.1) exists. Since G_N estimates G, we can write

$$G_N = G + \text{error}.$$

If the variance exists, the error appearing in the last statement is a random variable whose mean is 0 and whose width is characterized for large N by

$$|\text{error}| = \epsilon \cong \frac{\sigma_1}{N^{\frac{1}{2}}},$$

where

$$\sigma_1^2 = \int g^2(x) f(x)\, \mathrm{d}x - G^2. \tag{4.4}$$

The error estimate may be inverted to show the number of samples needed to yield a desired error, ϵ:

Monte Carlo Methods. Second Edition. M.H. Kalos and P.A. Whitlock

ISBN: 978-3-527-40760-6

$$N \cong \frac{\sigma_1^2}{\epsilon^2}. \tag{4.5}$$

The integral to be evaluated need not explicitly contain a function $f(x)$ satisfying the properties expressed by Equation 4.2. One can simply use $f(x) = 1/\Omega_0$ and $g(x) = \Omega_0 \times$ integrand instead. Later (cf. Equation 4.10 et seq.), we shall discuss more general ways of introducing a distribution function.

The integral in Equation 4.1 could also be evaluated by numerical quadrature. Let us assume that the domain of integration is an n-dimensional unit hypercube; then a numerical integration procedure can be written:

$$G \cong \sum w_i g(X_i) f(X_i),$$

where X_i is a lattice of points that fills the unit hypercube and w_i is a series of quadrature weights. The error associated with this quadrature is bounded by

$$\epsilon \leq ch^k, \tag{4.6}$$

where h measures the size of the interval separating the individual X_i. The constants c and k depend on the actual numerical integration method used, and k normally increases with more accurate rules. The bound on the error in Equation 4.6 is not a statistical variable, but is an absolute number. The actual error, however, is usually predictable to some degree.

If we assume that the time necessary for a computation, T_c will be proportional to the total number of points used, then

$$T_c \propto N = N_0 \left(\frac{1}{h}\right)^n, \tag{4.7}$$

where N_0 is a constant of the order of 1 and n is the number of dimensions. Equation 4.6 can be rewritten as

$$h \geq \left(\frac{\epsilon}{c}\right)^{\frac{1}{k}},$$

and Equation 4.7 becomes

$$\begin{aligned} T_c &\propto N_0 \left(\frac{c}{\epsilon}\right)^{\frac{n}{k}} \\ &= t_0 \epsilon^{\frac{-n}{k}}. \end{aligned} \tag{4.8}$$

The greater the accuracy demanded in a calculation, the greater the computational time will be.

In a Monte Carlo calculation, the total computation time is the product of the time t_2 for an individual sampling of times the total number of points;

$$T_c = t_1 N.$$

From Equation 4.5, this may be rewritten as

$$T_c = \frac{t_1\sigma_1^2}{\epsilon^2} = \frac{t_1'}{\epsilon^2};$$

the exponent of ϵ is the same in any number of dimensions. For large n, it is difficult to find a k in Equations 4.6 and 4.8 such that $n/k < 2$, so asymptotically, as $n \to \infty$, a Monte Carlo calculation is more advantageous than a numerical integration of Equation 4.1. The Monte Carlo calculation will take less total time for the same value of ϵ. This assumes that the two error estimates can be directly compared.

In spite of the apparently slow convergence ($\cong N^{-1/2}$) of the error of Monte Carlo quadrature, it is in fact more efficient computationally than finite difference methods in dimensions higher than 6–10.

Two different Monte Carlo evaluations of an integral can have differing variances. The quantity

$$Q_1 = t_1\sigma_1^2 \tag{4.9}$$

is a measure of the quality (efficiency) of a Monte Carlo calculation. The decision on which Monte Carlo algorithm to use in a large computation can be based on the values of Q_1 extracted from some trial calculations. A common phenomenon is for t to increase as σ decreases through a more elaborate Monte Carlo algorithm. The question is then whether the decrease in σ^2 will more than compensate for the increase in time. It will, if Q decreases.

Three major classes of techniques are used to reduce the variance in Monte Carlo quadrature:

1. Importance sampling can be introduced into the calculation to increase the likelihood of sampling variables where the function is large or rapidly varying.
2. The expected value of a random variable can be used rather than the variable itself. This substitution never increases variance and, many times, will substantially reduce it.
3. Correlations between succeeding samples may be exploited to advantage. In *control variates*, an easily evaluated approximation to the integrand is used to reduce the variance. If successive random variables are negatively correlated, the variance will be smaller than if they were independent. The technique called *antithetic variates* exploits the reduction in variance that results when negatively correlated samples are deliberately produced and grouped together.

4.1 Importance Sampling

Suppose we have an n-dimensional integral

$$G = \int g(x)f(x)\,\mathrm{d}x$$

that we wish to evaluate. The function $f(x)$ is not necessarily the best pdf to use in the Monte Carlo calculation even though it appears in the integrand. A different pdf, $\tilde{f}(x)$, can be introduced into the integral as follows:

$$G = \int \left[\frac{g(x)f(x)}{\tilde{f}(x)} \right] \tilde{f}(x)\, \mathrm{d}x, \tag{4.10}$$

where

$$\tilde{f}(x) \geq 0, \quad \int \tilde{f}(x)\, \mathrm{d}x = 1, \tag{4.11}$$

and $g(x)f(x)/\tilde{f}(x) < \infty$ except perhaps on a countable set of points. The variance of G when $\tilde{f}(x)$ is used becomes

$$\mathrm{var}\{G\}_{\tilde{f}} = \int \left[\frac{g^2(x)f^2(x)}{\tilde{f}^2(x)} \right] \tilde{f}(x)\, \mathrm{d}x - G^2. \tag{4.12}$$

G^2 being fixed, we want the $\tilde{f}(x)$ that will minimize the quantity $\int [g^2(x)f^2(x)/\tilde{f}(x)]\, \mathrm{d}x$. Of course, the integral is minimized by choosing $\tilde{f}(x)$ as large as we like, but we have the additional constraint expressed by Equation 4.11. The function $\tilde{f}(x)$ that satisfies the criteria given above may be deduced by using a Lagrange multiplier λ. In this method, we wish to find $\tilde{f}(x)$ such that

$$L\{\tilde{f}\} = \left[\int \frac{g^2(x)f^2(x)}{\tilde{f}(x)}\, \mathrm{d}x + \lambda \int \tilde{f}(x)\, \mathrm{d}x \right] \tag{4.13}$$

is minimized. We consider small variations of $\tilde{f}(x)$ on the quantity in brackets and set the variation of the quantity in brackets equal to zero

$$\frac{\delta}{\delta \tilde{f}}[\cdots] = 0.$$

Performing the functional differentiation yields

$$-\frac{g^2(x)f^2(x)}{\tilde{f}^2(x)} + \lambda = 0 \tag{4.14}$$

or

$$\tilde{f} = \lambda |g(x)f(x)|. \tag{4.15}$$

If the function $g(x)f(x)$ varied with x as the solid line in Figure 4.1, then $\tilde{f}(x)$ would be proportional to the dotted line. The value of λ may be found by requiring that $\int \tilde{f}(x)\, \mathrm{d}x = 1$. If $g(x) \geq 0$, then $\tilde{f}(x) = \lambda g(x)f(x)$ and $\lambda = 1/G$, so

$$\tilde{f}(x) = \frac{g(x)f(x)}{G}. \tag{4.16}$$

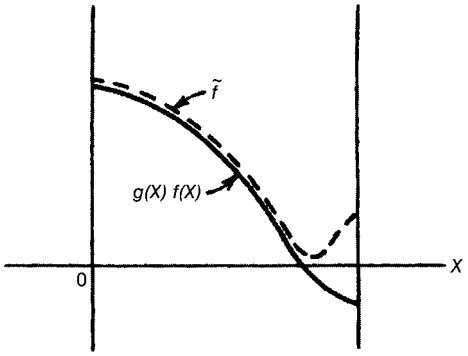


Figure 4.1 A function $g(X)f(X)$ and a possible $\tilde{f}$.

A Monte Carlo algorithm to evaluate the integral would be to sample a series of X_i from $\tilde{f}(x)$ and construct the sum

$$\tilde{G}_N = \frac{1}{N}\sum_{i=1}^{N}\frac{g(X_i)f(X_i)}{\tilde{f}(X_i)} = \frac{1}{N}\sum_{i=1}^{N}\frac{g(X_i)f(X_i)}{g(X_i)f(X_i)/G}$$

$$= \frac{1}{N}\sum_{i=1}^{N} G = G.$$

If we already know the correct answer G, the Monte Carlo calculation will certainly give it back with zero variance! This clearly corresponds to the minimum variance calculation. Although we cannot in practice use the $\tilde{f}(x)$ prescribed by Equation 4.16, we expect that ''similar'' functions will reduce the variance. What is meant will be explored in some examples. One important criterion is that $g(X_i)f(X_i)/\tilde{f}(X_i)$ be bounded from above.

As the first example, consider the integral

$$G = \int_0^1 \cos\left(\frac{\pi x}{2}\right) \mathrm{d}x.$$

A straightforward Monte Carlo algorithm would be to sample X_i uniformly on $(0, 1)$, ($f_1(x) = 1$), and to sum the quantity

$$g_1(x) = \cos\left(\frac{\pi x}{2}\right).$$

The variance of the population for a single sample of x may be analytically evaluated (Equation 4.4) and is

$$\mathrm{var}\{g_1\} = 0.0947\ldots.$$

By expanding $\cos(\pi x/2)$ in a power series, a better choice for the importance function may be found,

$$\cos\left(\frac{\pi x}{2}\right) = 1 - \frac{\pi^2 x^2}{8} + \frac{\pi^4 x^4}{2^4 4!} - \cdots$$

and we can let

$$\tilde{f}(x) = \frac{3}{2}\left(1 - x^2\right).$$

This pdf looks like the integrand for small values of x.[1)] The estimator for G is now

$$\tilde{g} = \frac{g_1}{\tilde{f}} = \frac{2}{3}\frac{\cos\left(\frac{\pi x}{2}\right)}{1 - x^2}$$

and the variance associated with a single sample is

$$\mathrm{var}\{\tilde{g}\} = 0.000990.$$

With this choice of importance function, the variance decreased by a factor of 100. As another example, consider the integral

$$\int_0^1 \sqrt{1 - x^2}\, \mathrm{d}x = \frac{\pi}{4};$$

again the straightforward Monte Carlo method would be to sample x uniformly on $(0, 1)$ and form the estimator

$$g_1 = \sqrt{1 - x^2}.$$

The variance associated with this procedure is

$$\mathrm{var}\{g_1\} = 0.050.$$

To improve the calculation, the integrand can be expanded in a power series about its maximum:

$$g = 1 - \frac{1}{2}x^2 + \cdots,$$

from which we infer that a reasonable importance function might be

$$\tilde{f}(x) = \frac{1 - \beta x^2}{1 - \frac{1}{3}\beta}. \tag{4.17}$$

The value of β may be chosen to give the minimum variance. With the choice of $\tilde{f}(x)$ given above, $\tilde{g}$ becomes

$$\tilde{g} = \frac{g_1}{\tilde{f}} = \left(1 - \frac{1}{3}\beta\right)\frac{\sqrt{1 - x^2}}{(1 - \beta x^2)}$$

and its variance is

$$\mathrm{var}\{\tilde{g}\} = \left(1 - \frac{1}{3}\beta\right)\left[\frac{1}{\beta} - \frac{(1 - \beta)}{\beta\sqrt{\beta}}\tanh^{-1}\sqrt{\beta}\right] - \left(\frac{\pi}{4}\right)^2.$$

1) It can be sampled by generating ξ_1 and ξ_2. If $\xi_2 \le \xi_1(3 - \xi_1)/2$, set $x = 1 - \xi_1$; otherwise set $x = \frac{1}{2}((9 - 8\xi_2)^{1/2} - 1)$.

Numerically minimizing the variance with respect to β gives $\text{var}\{\tilde{g}\} = 0.0029$ when $\beta = 0.74$. If we chose β to be $\frac{1}{2}$ as implied by the power series, the minimum variance is not achieved ($\text{var}\{\tilde{g}\} = 0.011$), but is still substantially lower than the variance associated with straightforward Monte Carlo. Very simple importance sampling schemes and ad hoc choices of parameters can lower the variance dramatically.

An experimental method of obtaining a parameter like β in an importance function is to try the Monte Carlo calculation with different values of β and estimate the value that minimizes the variance of $\tilde{g}$. The optimal value for β is not located precisely by this process because the fluctuations mask the trend, but we can hope that the variance of the Monte Carlo calculation is approximately constant in a neighborhood of the optimal β. A sample search for a good value of β is shown in Figure 4.2.

In a global sense, we want an importance function that matches the general behavior of the integrand at its maximum, but is also similar over the whole range of integration. In Figure 4.3, g is the integrand we wish to approximate. $\tilde{f}_1$ is an importance function derived from a Taylor series expansion; it is always greater than g. The function $\tilde{f}_2$ is a better importance function because it describes g better over the entire range of integration. In the previous example, the parameter β in Equation 4.17 could be chosen by letting

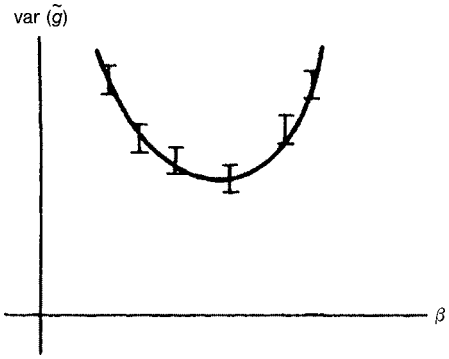


Figure 4.2 Finding the value of β that minimizes $\text{var}\{\tilde{g}\}$ graphically.

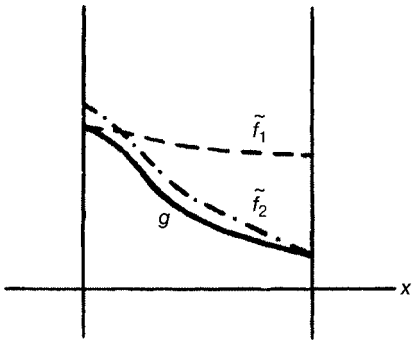


Figure 4.3 A function g and two possible importance functions $\tilde{f}_1$ and $\tilde{f}_2$.

$$1 - \beta x^2 = \sqrt{1 - x^2},$$

when $\sqrt{1 - x^2} = \frac{1}{2}$. The value of $\beta = \frac{2}{3}$ and the resulting variance of g is 0.0039, which is not much larger than the minimum variance. Therefore, it is not always necessary to calculate the variance as a function of β to select a β that substantially reduces the variance. Simple arguments of a dimensional type can locate the optimal β.

Singular Integrals

When the integrand $g(x)f(x)$ of an integral is singular, var$\{g(x)\}$ may not exist. In this case, we can always choose $\tilde{f}(x)$ such that the ratio $g(x)f(x)/\tilde{f}(x)$ is bounded. We assume here that $g(x)$ and $f(x)$ are known analytical functions whose singularities are easily identified. Consider the integral

$$\int \frac{dx}{x^{\frac{1}{2}}};$$

the straightforward Monte Carlo calculation would be to sample x uniformly on $(0, 1)$ with the estimator $g_1 = 1/x^{1/2}$. The variance contains $\langle g^2 \rangle$, which is

$$\langle g^2 \rangle = \int_0^1 \frac{dx}{x} = \infty,$$

so that the variance for this calculation does not exist. As an alternative, we can try

$$\tilde{f}(x) = (1 - u)x^{-u},$$

where $u < 1$. The estimator for G is now

$$\tilde{g} = \frac{x^{u-\frac{1}{2}}}{1 - u},$$

and the nth moment of $\tilde{g}$ is

$$\langle \tilde{g}^n \rangle = (1 - u)^{-n+1} \int_0^1 x^{nu-\frac{n}{2}} x^{-u}\, dx.$$

For the integrals to exist,

$$(n - 1)u - \frac{n}{2} > -1,$$

and, in particular, all moments will exist if $1 > u \geq \frac{1}{2}$. Of course, the optimal u is $u = \frac{1}{2}$.

As a second example, suppose we wish to evaluate

$$\int_0^1 \frac{dx}{[x(1 - x)]^{\frac{1}{2}}};$$

again, a straightforward Monte Carlo calculation will have an infinite variance. To eliminate this, we shall introduce an $\tilde{f}(x)$ that has singularities both at 0 and at 1:

$$\tilde{f}(x) = \frac{1}{4\sqrt{x}} + \frac{1}{4\sqrt{1-x}}.$$

The method for sampling $\tilde{f}(x)$ was described in Section 3.4.4. The estimator $\tilde{g}(x)$ becomes

$$\tilde{g}(x) = \frac{\dfrac{4}{\sqrt{x(1-x)}}}{\dfrac{1}{\sqrt{x}} + \dfrac{1}{\sqrt{(1-x)}}} = \frac{4}{\sqrt{x} + \sqrt{(1-x)}}.$$

$\tilde{g}(x)$ is bounded by 4 from above and is greater than $4/\sqrt{2}$ (Figure 4.4). The variance associated with $\tilde{g}(x)$ is easily bounded:

$$\text{var}\{\tilde{g}\} = \int \tilde{f}(x)(\tilde{g} - G)^2 \, dx < \left(4 - \frac{4}{\sqrt{2}}\right)^2 = 1.37,$$

and we have eliminated the infinite variance.

The strategy needed to develop an importance function is to identify the singularities, i.e.

$$g(x) \cong \begin{cases} x^{\frac{-1}{2}} & \text{near } x = 0 \\ (1-x)^{\frac{-1}{2}} & \text{near } x = 1, \end{cases}$$

and simply take a sum of the singularities as the importance function. From the composition method (Section 3.4), we know we can sample the sum. It is not really necessary to discuss exotic central limit theorems in Monte Carlo calculations, since we can always eliminate infinite variances through importance sampling.

As a last example, we shall evaluate a singular integral of some practical interest. Let $\mathbf{X}$ and $\mathbf{X}_0$ be three-dimensional vectors contained in the volume $\mathbf{V}$ and $S(\mathbf{X})$ a function bounded away from zero and infinity, $0 < S_0 \leq S(\mathbf{X}) < S_1 < \infty$. Consider the integral

$$\langle S \rangle = \int_{\mathrm{V}} \frac{S(\mathbf{X}) \exp(-\mu |\mathbf{X} - \mathbf{X}_0|)}{|\mathbf{X} - \mathbf{X}_0|^2} \, d\mathbf{X}, \tag{4.18}$$

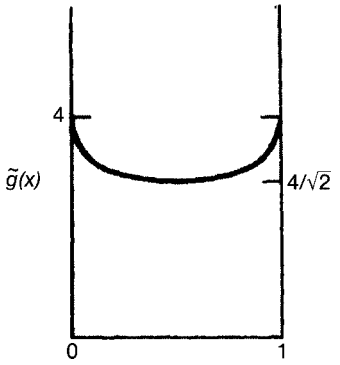


Figure 4.4 The estimator $\tilde{g}(x)$ as a function of x.

where

$$\int_{\mathbf{V}} S(\mathbf{X})\, d\mathbf{X} = 1.$$

Physically, this integral occurs in the neutral radiation transport problem with source $S(\mathbf{X})$, attenuation with coefficient μ, and an infinitesimal detector at $\mathbf{X}_0$. The "natural" way to evaluate Equation 4.18 is to sample $\mathbf{X}$ from $S(\mathbf{X})$ and sum the quantity

$$g(\mathbf{X}) = \frac{\exp(-\mu|\mathbf{X} - \mathbf{X}_0|)}{|\mathbf{X} - \mathbf{X}_0|^2}. \tag{4.19}$$

We make a change of the coordinates by letting $\mathbf{X} - \mathbf{X}_0 = \mathbf{r}$. $d\mathbf{X} = d\mathbf{r}$ since $\mathbf{X}_0$ is fixed. The integral then becomes

$$\langle S \rangle = \int_{\mathbf{V}} S(\mathbf{r} + \mathbf{X}_0) \frac{\exp(-\mu r)}{r^2}\, d\mathbf{r}. \tag{4.20}$$

The variance associated with the estimator of the integral in Equation 4.19 will contain the quantity

$$\langle g^2 \rangle = \int_{\mathbf{V}} S(\mathbf{r} + \mathbf{X}_0) \frac{\exp(-\mu r)}{r^4}\, d\mathbf{r};$$

we may bound $\langle g^2 \rangle$ by invoking the integral theorem of the mean. Since $S(\mathbf{X})$ is bounded away from 0,

$$\langle g^2 \rangle \geq S_0 \int_{\mathbf{V}} \frac{\exp(-2\mu r)}{r^4}\, d\mathbf{r};$$

this is less than the integral over the largest sphere wholly contained in $\mathbf{V}$

$$\langle g^2 \rangle \geq 4\pi S_0 \int \frac{\exp(-2\mu r)}{r^4} r^2\, dr, \tag{4.21}$$

which diverges. Therefore the variance does not exist for the estimator in Equation 4.19.

To have a finite-variance Monte Carlo calculation, we must change the method of sampling. Suppose that b is the radius of the smallest sphere centered at $\mathbf{X}_0$ that contains $\mathbf{V}$; we can introduce a pdf, $f(\mathbf{r})$, for sampling within the sphere as

$$f(\mathbf{r}) = \frac{\mu}{4\pi[1 - \exp(-\mu b)]} \frac{\exp(-\mu r)}{r^2}. \tag{4.22}$$

To sample an $\mathbf{r}$ we write $f(\mathbf{r})\, d\mathbf{r}$ as

$$f(\mathbf{r})\, d\mathbf{r} = f(r) r^2\, dr \sin\theta\, d\theta\, d\phi \tag{4.23}$$

$$= \frac{\mu \exp(-\mu r)}{[1 - \exp(-\mu b)]}\, dr \frac{\sin\theta\, d\theta}{2} \frac{d\phi}{2\pi}. \tag{4.24}$$

Sample $\cos\theta$ uniformly on $(-1, 1)$ and ϕ uniformly on $(0, 2\pi)$. If b were infinite, the r function would be $\mu \exp(-\mu r)\, dr$, which can be sampled by $r = -(1/\mu)\log\xi$. For finite b, $\mu \exp(-\mu r)/[1 - \exp(-\mu b)]$ may be sampled by setting

$$r = -\frac{1}{\mu}\log\xi \pmod{b}. \tag{4.25}$$

Using $f(\mathbf{r})$ in Equation 4.22, the integral in Equation 4.18 becomes

$$\langle S\rangle = \frac{[1-\exp(-\mu b)]4\pi}{\mu}\int_{\mathrm{V}} S(\mathbf{r}+\mathbf{X}_0)f(\mathbf{r})\,\mathrm{d}\mathbf{r}$$

and the estimator for $\langle S\rangle$ is

$$\tilde{g}(\mathbf{r}) = \frac{[1-\exp(-\mu b)]4\pi}{\mu}S(\mathbf{r}+\mathbf{X}_0).$$

The variance contains $\langle\tilde{g}^2\rangle$,

$$\langle\tilde{g}^2\rangle = \left(\frac{[1-\exp(-\mu b)]}{\mu}4\pi\right)^2\int S^2(\mathbf{r}+\mathbf{X}_0)f(\mathbf{r})\,\mathrm{d}\mathbf{r}.$$

This can be bounded by

$$\langle\tilde{g}^2\rangle \le \left(\frac{1-\exp(-\mu b)}{\mu}4\pi\right)^2 S_1^2\int f(\mathbf{r})\,\mathrm{d}\mathbf{r}. \tag{4.26}$$

Since $\int f(\mathbf{r})\,\mathrm{d}\mathbf{r} = 1$, the variance exists.

The actual Monte Carlo algorithm will comprise sampling an $\mathbf{r}$ from $f(\mathbf{r})$; if $\mathbf{r}+\mathbf{X}_0$ is outside the volume $\mathbf{V}$ the contribution of $S(\mathbf{r}+\mathbf{X}_0)$ will be zero. The value of the variance obtained in the calculation will be adversely affected by many zeros occurring in the estimate for $\langle S\rangle$. If a pdf defined within a sphere containing $\mathbf{V}$ proves to be unsuitable in the calculation because of frequent sampling of $\mathbf{r}$ outside $\mathbf{V}$, it may be necessary to design a rejection technique for $f(\mathbf{r})$ that is nonzero only within $\mathbf{V}$ or to sample $\mathbf{r}$ from Equation 4.22 over a smaller sphere and use a different distribution in the rest of $\mathbf{V}$.

Importance sampling is a very useful technique for reducing variance and for handling singular integrals. It will be used repeatedly in the applications of Monte Carlo methods to be discussed. A shortcoming of importance sampling is that it is difficult to apply if the integrand changes sign. In such cases, it will normally be advantageous to use correlated sampling methods, Section 4.3.

Importance Sampling with Correlated Sampling

Suppose we need to evaluate the integrals

$$G_n = \int g_n(x)f(x)\,\mathrm{d}x, \tag{4.27}$$

where the $g_n(x), n = 1, 2, \ldots, M$, are a sequence of functions. The most direct method would be to sample an x_i from $f(x)$ and evaluate all the functions for the particular x_i and repeat the process as many times as necessary; that is, sample $x_1, \ldots, x_N$ and form

$$G_{nN}.. = \frac{1}{N}\sum_{i=1}^{N} g_n(x_i).$$

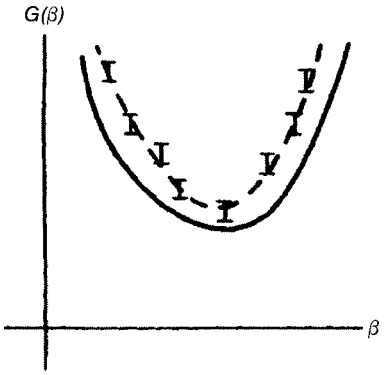


Figure 4.5 Using positive correlation to locate the minimum of an integral $G(\beta)$.

It is also possible to introduce importance sampling into the integral,

$$G_n = \int \frac{g_n(x)f(x)}{\tilde{f}(x)}\tilde{f}(x)\,dx,$$

sample an x_i from $\tilde{f}(x)$ and form

$$G_{nN} = \frac{1}{N}\sum_{i=1}^{N}\frac{g_n(x_i)f(x_i)}{\tilde{f}(x_i)}.$$

By using the same x_i for all the $g_n(x)$ saves computer time in sampling $f(x)$ or $\tilde{f}(x)$. In many cases, the $g_n(x)$ will not differ much; for example, a parameter in the analytical expression for $g_n(x)$ may be changed to observe systematic variations. Positive correlation is introduced into the estimates for G_n by using the same x_i and random fluctuations are eliminated. If we were searching for the parameter β that minimizes the integral $G(\beta)$, the positive correlation makes it easier to locate the minimum β (Figure 4.5).

4.2
The Use of Expected Values to Reduce Variance

The following discussion describes the use of expected values in finite quadrature but its application is much more wide ranging.

Suppose we wish to evaluate the integral

$$G = \int g(x,y)f(x,y)\,dx\,dy, \tag{4.28}$$

where x and y may be many-dimensional vectors (though Y is usually one-dimensional). The marginal distribution for x is defined by Equation 2.32

$$m(x) = \int f(x,y)\,dy, \tag{4.29}$$

and we can define another quantity $h(x)$ as

$$h(x) = \frac{1}{m(x)} \int g(x, y) f(x, y)\, dy. \tag{4.30}$$

We assume that the integrals $m(x)$ and $h(x)$ can be evaluated by means other than Monte Carlo. The integral in Equation 4.28 can be rewritten

$$G = \int m(x) h(x)\, dx. \tag{4.31}$$

We further assume that the order of integration is immaterial. The difference in variance between Equations 4.28 and 4.31 is (cf. Section 2.5)

$$\begin{aligned} \text{var}\{g\} - \text{var}\{h\} &= E(g^2) - E((E(g|x))^2) \\ &= E(E(g^2|x)) - E((E(g|x))^2) \\ &= E(E(g^2|x) - (E(g|x))^2) = E(\text{var}\{g|x\}) \geq 0 \end{aligned} \tag{4.32}$$

and we have shown the general theorem that

$$\text{var}\{g(x, y)\} - \text{var}\{h(x)\} \geq 0. \tag{4.33}$$

In other words, the variance of a Monte Carlo calculation may be reduced by doing part of the integration analytically as in Equation 4.30.

As an example, consider the integral

$$\frac{\pi}{4} = \int_0^1 \int_0^1 g(x, y)\, dx\, dy,$$

where

$$g(x, y) = \begin{cases} 1, & x^2 + y^2 \leq 1 \\ 0, & x^2 + y^2 > 1. \end{cases}$$

If we choose x and y uniformly within the unit square and sum $g(x, y)$, the variance associated with the Monte Carlo estimator is

$$\text{var}\{g\} = \frac{\pi}{4} - \left(\frac{\pi}{4}\right)^2 = 0.168.$$

Instead, we can evaluate the marginal distribution for x,

$$m(x) = \int_0^1 dy = 1,$$

and define the quantity $h(x)$ by

$$h(x) = \frac{1}{m(x)} \int g(x, y) f(x, y)\, dy = \int_0^{\sqrt{1-x^2}} dy = \sqrt{1 - x^2}.$$

The integral is rewritten

$$G = \int_0^1 \sqrt{1 - x^2}\, \mathrm{d}x.$$

A Monte Carlo algorithm would be to sample x uniformly on $(0, 1)$ and sum the $h(x)$. The variance associated with this is

$$\mathrm{var}\{h\} = \int_0^1 (1 - x^2)\, \mathrm{d}x - \left(\frac{\pi}{4}\right)^2 = 0.050,$$

which is indeed a reduction over the previous value. The improvement in the variance will be lost, however, if the second method takes much longer to compute (here, the time for calculation of the square root). The computational time for fixed error can be decreased by using importance sampling to improve the sampling of $\sqrt{1 - x^2}$; the calculation would then be a combination of expected values and importance sampling. To use the expected value of the random variable in the Monte Carlo calculation, it must be possible to evaluate $m(x)$ analytically.

Expected Values in M(RT)^2

Expected values can also be advantageously applied to the Metropolis *et al.* method. As described previously in Section 3.7, the M(RT)^2 technique generates a random walk in which a possible next step X'_{n+1} is sampled from the transition distribution $T(X'_{n+1}|X_n)$. The probability of accepting the new step is given by

$$A(X'_{n+1}|X_n) = \min\left[1, \frac{f(X'_{n+1})T(X_n|X'_{n+1})}{f(X_n)T(X'_{n+1}|X_n)}\right]$$

and $X_{n+1} = X'_{n+1}$ with probability $A(X'_{n+1}|X_n)$ and $X_{n+1} = X_n$ with probability $1 - A(X'_{n+1}|X_n)$. The method guarantees that the asymptotic distribution of the X_i will be $f(X)$. To estimate a quantity G,

$$G = \int g(X) f(X)\, \mathrm{d}X,$$

$$G \cong \frac{1}{N} \sum g(X_i),$$

the $g(X_i)$ are summed only after the asymptotic distribution, $f(X)$, has been attained in the random walk. Suppose that we are at step X_n in the random walk and have sampled a possible next step X'. Conditional on X_n, the expectation value for $g(X_{n+1})$ is

$$E(g(X_{n+1})) = \int_0^1 \int_0^1 g_1(X', \eta) T(X'|X_n)\, \mathrm{d}X'\, \mathrm{d}\eta,$$

where

$$g_1(X', \eta) = \begin{cases} g(X') & \text{if } \eta \le A(X'|X_n) \\ g(X_n) & \text{if } \eta > A(X'|X_n). \end{cases}$$

The variable η is a uniform random variable and the Monte Carlo calculation may be improved by using its expected value in the algorithm. The marginal distribution for X' is

$$m(X') = \int_0^1 T(X'|X_n)\, d\eta = T(X'|X_n)$$

and $h(X')$ becomes from Equation 4.30

$$\begin{aligned} h(X') &= \frac{1}{T(X'|X_n)} \int_0^1 g_1(X', \eta) T(X'|X_n)\, d\eta \\ &= \frac{1}{T(X'|X_n)} \left[\int_0^A g(X') T(X'|X_n)\, d\eta + \int_A^1 g(X_n) T(X'|X_n)\, d\eta \right] \\ &= g(X') A(X'|X_n) + g(X_n) \left[1 - A(X'|X_n) \right]. \end{aligned}$$

That is, the scores at X' and X_n are weighted with the probabilities that X' or X_n will be the next point.

In some applications, $A(X'|X_n)$ is either 0 or 1 (e.g. in sampling classical many-body systems with hard sphere forces), so there is no advantage in using expected values. There are many applications in which $A(X'|X_n)$ varies smoothly between 0 and 1 and the method can be very useful. Usually, the most computer time in an $M(RT)^2$ algorithm is spent calculating $f(X')$ and $f(X_n)$ for the acceptance probability. The calculation becomes more efficient if $g(X')$ and $g(X_n)$ are determined simultaneously with $f(X')$ and $f(X_n)$. In conventional $M(RT)^2$ applications, one of the quantities, $g(X)$ or $g(X_n)$, is then thrown away, whereas if expected values are used, both values are needed. In the earlier example of disks in a box, $f(X)$ is determined by checking whether any disks overlap or are outside the box. Since all separations of pairs of disks must be calculated for $f(X)$, it is most efficient to keep track of the occurrences of a particular separation [which is $g(X)$] at the same time. The expected values method will be useful if the disks are not subject to perfect repulsion and especially if $g(X)$ is sensitive to the effects of small distances.

4.3
Correlation Methods for Variance Reduction

Correlation methods serve to reduce the variance by the use of correlated points in the sampling rather than sampling all points independently. In a technique called *control variates* [1], the integral of interest,

$$G = \int g(x) f(x)\, dx$$

is written

$$G = \int (g(x) - h(x)) f(x)\, dx + \int h(x) f(x)\, dx, \tag{4.34}$$

where $\int h(x)f(x)\,dx$ is known analytically. The estimator for G becomes

$$G \cong \int h(x)f(x)\,dx + \frac{1}{N}\sum_{i=1}^{N}[g(x_i) - h(x_i)], \tag{4.35}$$

with $g(x)$ and $h(x)$ evaluated at the same points (x_i). The technique is advantageous when

$$\mathrm{var}\{(g(x) - h(x))\}_f \ll \mathrm{var}\{g(x)\}_f, \tag{4.36}$$

and this occurs when $h(x)$ is very similar to $g(x)$. If $\int g(x)f(x)\,dx$ closely resembles a known integral, then the method will probably be useful. In particular, if $|g(x) - h(x)|$ is approximately constant for different values of $h(x)$, then correlated sampling will be more efficient than importance sampling [2]. Conversely, if $|g(x) - h(x)|$ is approximately proportional to $|h(x)|$, then importance sampling would be the appropriate method to use.

Consider the integral

$$\int_0^1 e^x\,dx,$$

a straightforward Monte Carlo calculation gives a variance equal to 0.242. A possible $h(x)$ derives from the first two terms in the Taylor series expansion for e^x,

$$\int_0^1 e^x\,dx = \int_0^1 (e^x - (1 + x))\,dx + \frac{3}{2},$$

where $\int_0^1 (1 + x)\,dx = \frac{3}{2}$. The random variable x may be chosen uniformly on $(0, 1)$ and the associated variance is

$$\mathrm{var}\{e^x - (1 + x)\} = 0.0437,$$

which is a substantial reduction from the variance quoted above. By using $\frac{2}{3}(1 + x)$ as an importance function, however, the variance is decreased to 0.0269.

As a better example, consider the integral

$$\int_0^1 (e^x - (1 + \beta x))\,dx,$$

where we shall minimize the variance with respect to β. We want the value of β for which

$$\int_0^1 (e^x - 1 - \beta x)^2\,dx - \left(\int_0^1 (e^x - 1 - \beta x)\,dx\right)^2$$

is smallest. Experimentally it can be determined that $\beta = 1.69$ gives a variance of 0.0039. The best fit to the exponential in the sense given here is not far from the best fit for a straight-line importance function. In the latter case, $\beta = 1.81$ is optimal and the variance is 0.0040, rather close to the best value found here.

In practice, the experimental determination of an optimal parameter or parameters for a control variate treatment of a many-dimensional integral cannot be carried out with great precision, since determination of the variance to be minimized must itself be determined by Monte Carlo.

Control variates are used extensively in simulations [3], particularly in the study of queues and queuing networks.

4.3.1 Antithetic Variates

The method of antithetic variates [4] exploits the decrease in variance that occurs when random variables are negatively correlated. When variables are negatively correlated, if the first point gives a value of the integrand that is larger than average, the next point will be likely to give a value that is smaller than average, and the average of the two values will be closer to the actual mean. In theory, the method sounds promising, but in practice it has not been very successful as a general variance reduction method in many dimensions [5]. It can often be used to advantage for a few variables of the many [6].

Suppose that

$$G = \int_0^1 g(x)\,\mathrm{d}x, \tag{4.37}$$

where $g(x)$ is linear. Then G may be written exactly as

$$G = \int_0^1 \frac{1}{2}[g(x) + g(1-x)]\,\mathrm{d}x. \tag{4.38}$$

G may be evaluated through Monte Carlo by using Equation 4.38 and picking an x uniformly on $(0, 1)$. The value of $g(x)$ and $g(1-x)$ is determined and the estimate for G formed,

$$G_N = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{2}[g(x_i) + g(1-x_i)], \tag{4.39}$$

which will give exactly G with zero variance for linear g (Figure 4.6). For nearly linear functions, this method will substantially reduce the variance.

Consider the integral discussed earlier,

$$G = \int_0^1 \mathrm{e}^{-x}\,\mathrm{d}x;$$

the variance associated with a straightforward Monte Carlo evaluation is 0.242. If we pick x_i uniformly and at random on $(0, 1)$ and form the estimator in Equation 4.39

$$G_N = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{2}\left[g(x_i) + g(1-x_i)\right];$$

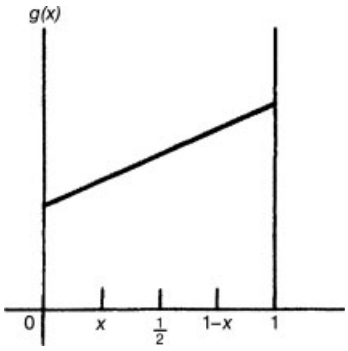


Figure 4.6 A linear function $g(x)$ on $(0, 1)$.

the variance associated with this calculation is 0.0039, which is a dramatic reduction in variance.

As another example, take

$$G = \int_0^\infty e^{-x} g(x)\, dx.$$

We shall use e^{-x} as the sampling function. A random number distributed exponentially is given by

$$x = -\log \xi.$$

A correlated random variable is $x' = -\log(1 - \xi)$. If x is close to the origin, x' will be far from the origin. The values for x and x' can be substituted in the expression for the estimator in Equation 4.39, which becomes

$$G = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2} \left\{ g(x_i) + g(x_i') \right\}.$$

This will be an improvement over the use of a single estimate if g is monotone. Two generalizations of Equation 4.39 may be introduced, for any $0 < \alpha < 1$:

$$g_{+\alpha} = \{\alpha g(\alpha x) + (1 - \alpha) g(\alpha + (1 - \alpha)x)\}$$

and (4.40)

$$g_{-\alpha} = \{\alpha g(\alpha x) + (1 - \alpha) g(1 - (1 - \alpha)x)\};$$

these functions are linear and have the correct expectation. A value for α may be established by solving

$$g_{-\alpha}(0) = g_{-\alpha}(1),$$

$$g(\alpha) = (1 - \alpha) g(1) + \alpha g(0). \tag{4.41}$$

Correlation techniques need not be used alone, but may be combined with other methods of reducing the variance. For example, both importance sampling and

antithetic variables may be used simultaneously to improve a calculation. Thus the result expressed in Equation 4.38 may be improved by importance sampling as

$$G = \frac{1}{2}\int_0^1 \left[\frac{g(x) + g(1-x)}{\tilde{f}(x)}\right]\tilde{f}(x)\,dx. \tag{4.42}$$

Consider again $\int_0^1 e^x\,dx$. The antithetic estimator $\frac{1}{2}[e^x + e^{1-x}]$ is symmetric about $x = \frac{1}{2}$, so an approximate $\tilde{f}$ for this problem is

$$\tilde{f}(x) = \frac{24}{25}\left[1 + \frac{1}{2}\left(x - \frac{1}{2}\right)^2\right],$$

chosen to agree with the first three terms of the power series at $x = \frac{1}{2}$. The variance of the estimator of Equation 4.42 with this sampling function is 0.0000012, compared with 0.0039 for the estimator of Equation 4.38 and 0.242 for the straightforward evaluation. Thus, use of antithetic variates reduces the variance by 2 orders of magnitude, and this simple unoptimized importance sampling by another three!

4.3.2 Stratification Methods

In stratification methods, the domain of the independent variable is broken up into subintervals such that a random variable is sampled from every subinterval. For the one-dimensional integral

$$G = \int_0^1 g(x)\,dx, \tag{4.43}$$

the simplest stratification is to divide $(0, 1)$ into M equal intervals. An x is then chosen in each interval in succession,

$$x_j = \frac{\ell - \xi_j}{M},$$

where $\ell = (j-1) \pmod M + 1$ and $j = 1, 2, \ldots, NM$. The ℓ's will cycle through the integer values 1 through M, and the x_j will be drawn at random in the ℓth interval. An estimator for G is given by

$$G_{NM} = \frac{1}{NM}\sum_{j=1}^{M} g(x_j). \tag{4.44}$$

It is best, however, not to use Equation 4.44 as written, since estimation of the variance is difficult. Rewriting G_{NM} as

$$G_{NM} = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{1}{M}\sum_{j=1}^{M} g(x_j)\right),$$

gives terms $(1/M)\sum_{j=1}^{M} g(x_j)$ that are statistically independent. The variance is straightforward to calculate from these. In correlation methods, it is very important

to group answers such that the individual groups are independent in order to calculate the variance. For example, in antithetic variates, we group two (or more) answers as an independent estimate in the determination of the variance.

An alternative method for stratifying the sampling of an x for the integral in Equation 4.43 would be to use the same random number in each subinterval per cycle of ℓ. That is

$$x_j = \frac{\ell - \xi_k}{M},$$

where

$$\ell = (j-1)(\text{mod } M) + 1,$$
$$k = \left[\frac{j-1}{M}\right] + 1,$$

and $j = 1, \ldots, M$. In one dimension, this is analogous to trapezoidal integration, but the random choice of x on a subinterval removes a bias.

There is no particular reason for choosing the subintervals to be of equal size. An estimator g_k for the integral in Equation 4.43 can be defined that allows varying subinterval size,

$$g_k = \sum_{j=1}^{k} \sum_{i=1}^{n_j} (\alpha_j - \alpha_{j-1}) \frac{1}{n_j} g[\alpha_{j-1} + (\alpha_j - \alpha_{j-1})\xi_{ij}]. \tag{4.45}$$

The notation ξ_{ij}, indicates that a new random number is chosen for every combination of (i,j); the random number is then mapped onto the interval (α_{j-1}, α_j) in which n_j samples are to be drawn. The sampling algorithm maps (i,j) onto the interval (α_{j-1}, α_j). A particular subinterval (α_{j-1}, α_j) is sampled n_j times, and the mean of the g's evaluated within (α_{j-1}, α_j) is multiplied by the size of the interval. This is a generalization of the trapezoidal rule for integration since the size of the interval changes. The variance on a subinterval is proportional to the number of samples taken within the subinterval

$$n_j^2 \propto \left\{ (\alpha_j - \alpha_{j-1}) \int_{\alpha_{j-1}}^{\alpha_j} g^2(x)\, \mathrm{d}x - \left[\int_{\alpha_{j-1}}^{\alpha_j} g(x)\, \mathrm{d}x \right]^2 \right\}.$$

It is possible to minimize the variance with respect to n_j to determine the optimal value of n_j.

It is not really necessary to use variable interval size stratified sampling, since an importance sampling transformation will achieve the same goal. The motivation to vary the subinterval size is to have large intervals where the function is nearly constant and fine intervals where the function is large or rapidly changing. But importance sampling leads to the same result by sampling a function that is large where f is large. A useful approach is to importance-sample an integral and then use stratified sampling on the transformed integral.

A straightforward generalization of stratified sampling to many dimensions is not efficient, since it leads to the necessity of sampling in many cells. Rather than attempt to stratify all the dimensions, it is better to identify which variables (if any) carry most of the variation of the integrand and stratify these. Significant reduction in the variance can sometimes be achieved by stratifying a single dimension in a many-dimensional integral. An alternative approach is to use an adaptive Monte Carlo method to concentrate the sampling in the most important regions, Section 4.4.

Suppose we wish to sample random variables from the unit square in two dimensions. The generalization of simple stratification into four intervals in one dimension would be to divide the square into 16 subintervals and sample a point in each box (Figure 4.7). An alternative of this has been suggested by (H.A. Steinberg, private communication), in which points are sampled in only four boxes, one from each row. The points would be chosen in boxes $(1, n_1)$, $(2, n_2)$, $(3, n_3)$, $(4, n_4)$, where the sequence n_1, n_2, n_3, n_4 is a random permutation of $1, 2, 3, 4$. A particular permutation of the sequence is shown in Figure 4.8. The sampled boxes will stay apart in this scheme, and no accidental sampling of two random variables in the same subinterval will occur. We see that it is always perfectly stratified with respect

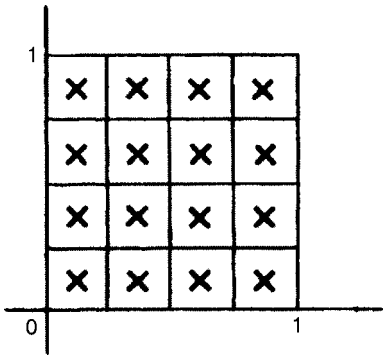


Figure 4.7 Dividing the unit square into 16 subintervals.

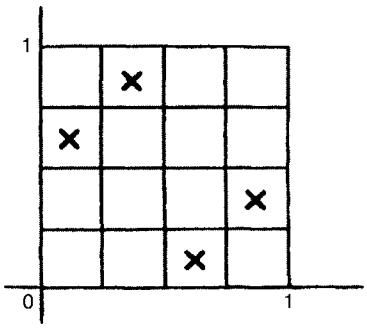


Figure 4.8 Sampling one subinterval from each row in the unit square by a random permutation.

to x and y separately, which is better than arbitrarily choosing a single direction and then stratifying. In two dimensions, Steinberg's scheme is not usually an improvement, but its generalization to many dimensions permits the retention of much of the advantage of stratification with reasonably small groups of correlated variables.

Specifically, suppose we wish to stratify k samples in a d-dimensional unit hypercube. Let each of the sides be divided into k segments (for a total of k^d small hypercubes). Form $d-1$ independent permutations of the integers $1, 2, \ldots, k$. Let the ith members of the jth permutation be $n(i, j)$. Assemble k d-tuples as

$$
\begin{aligned}
&[1, n(1,1), n(1,2), n(1,3), \ldots, n(1, d-1)],\\
&[2, n(2,1), n(2,2), n(2,3), \ldots, n(2, d-1)],\\
&\quad\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\\
&[k, n(k,1), n(k,2), n(k,3), \ldots, n(k, d-1)],
\end{aligned}
$$

and place a sample at a point in each of the small hypercubes so defined. As before, the points can but need not be independently sampled within each hypercube.

4.4 Adaptive Monte Carlo Methods

Similar to other variance reduction techniques, adaptive Monte Carlo (AMC) methods seek to concentrate the computational effort in the regions where the integrand is varying most and thereby reduce the variance. Instead of sampling random variables uniformly within the domain, in AMC methods the domain is partitioned into a subdivision tree that is based on the behavior of the integrand. In the simplest adaptive schemes, the original domain of integration is divided into a small number of partitions, and Monte Carlo integration is performed separately in each of these smaller subregions to yield an estimate of the integral in the subdomain and its associated error. Assuming that the errors are not acceptable, the subdomains are further partitioned. The subdivision process can be based on purely local information or take global behavior into account. For example, a locally based process could compare the error within each subdomain to a stopping criteria and if an error is too large, the associated subdomain is split into two smaller partitions. The Monte Carlo evaluation of the integral is then performed in the smaller partitions. An iterative process is continued until all the subdomain errors are acceptable. An alternative global strategy would be to compare the statistical errors in all the subdomains. The subdomain with the largest error is then split into two smaller subdomains. Each iteration of the algorithm leads to the partition of the subdomain with the largest error. The process continues until the overall error has satisfied the stopping criteria or a predetermined number of iterations have been completed.

A description of the global adaptive process is given below:

1. Divide the domain into initial subdomains.
2. Perform Monte Carlo integration in each subdomain and calculate the error.

3. Choose the subdomain with the largest error and divide the region into two parts. Perform the Monte Carlo integrations in the new subdomains and calculate the errors.
4. Store the new subdomains.
5. Calculate the overall error. If it is acceptable or the maximum number of iterations has been exceeded, stop the calculation. Else return to step 3.

In the previous discussion, using either local or global information, the subdomains were split into smaller divisions of equal size. In superconvergent adaptive Monte Carlo (SAMC), information about the integrand can be used to choose the size of the subdomains and hasten convergence. The ideas motivating SAMC can be demonstrated by a one-dimensional example.

Let the domain of integration, Ω_0, of Equation 4.1 be $[0, 1]$ and partition this interval into m subintervals, Ω_i, guided by the behavior of $g(x)$, $x_0 = 0$, $x_m = 1$;

$$C_i = \frac{1}{2}\left[g(x_{i-1}) + g(1)\right](1 - x_{i-1}),\ i = 1, \ldots, m-1,$$

$$x_i = x_{i-1} + \frac{C_i}{g(x_{i-1})(n - i + 1)}$$

with $\Omega_i \equiv [x_{i-1}, x_i]$. The integral in Equation 4.1 can be rewritten as

$$G = \int_0^1 g(x)f(x)\,\mathrm{d}x = \sum_{i=1}^{m} \int_{x_{i-1}}^{x_i} g(x)f(x)\,\mathrm{d}x.$$

To evaluate G by SAMC, let,

$$f_i = \int_{x_{i-1}}^{x_i} f(x)\,\mathrm{d}x \quad \text{and} \quad G_i = \int_{x_{i-1}}^{x_i} g(x)f(x)\,\mathrm{d}x.$$

Then, n_i random variables, X_j^i can be sampled on each Ω_i from $f(x)/f_i$ and the estimator for G_i formed,

$$G_i = E\left(\frac{f_i}{n_i}\sum_{j=1}^{n_i} g(X_j^i)\right)$$

and their associated statistical errors evaluated. The integral is evaluated as

$$G = E\left(\sum_{i=1}^{m}\frac{f_i}{n_i}\sum_{j=1}^{n_i} g(X_j^i)\right),$$

where $n = \sum_{i=1}^{m} n_i$ is the overall number of points sampled at a single iteration. The iterations proceed as before until some stopping criteria is satisfied.

It can be shown that the probable error of the SAMC algorithm decreases as $cn^{-(1/2)-(1/d)}$ [7] where d is the dimensionality of the integral. Eventually, as the dimensionality increases, the SAMC method will offer no advantage over the simpler AMC method.

4.5 Quasi-Monte Carlo

An alternative technique to evaluate integrals and integral equations, labeled quasi-Monte Carlo (q-MC), uses deterministic sequences of variables that are particularly well distributed. The one dimensional integral,

$$G = \int_0^1 g(x)\, \mathrm{d}x \tag{4.46}$$

is still estimated by

$$G_N = \frac{1}{N}\sum_{i=1}^{N} g(x_i); \tag{4.47}$$

however, the sequence $x_1, \ldots, x_N$, is chosen in such a way that the quantity, $|G_N - G|$, is minimized. Bounds on $|G_N - G|$ can be developed and lead to the definition of the discrepancy, D_N^*, for a set of N numbers.

Let $x_1, \ldots, x_N$ be a sequence of N numbers in $I = [0, 1]$ and S be a subset of I. Define $V_N(S)$ to be the proportion of the x_i, $1 \le i \le N$, that are within S and further define $\Delta_N(S) = V_N(S) - \text{length}(S)$. Then it can be shown that if $g(x)$ is Riemann-integrable [8],

$$\begin{aligned} |G_N - G| &= \left| \int_0^1 \Delta_N([0, x])\, \mathrm{d}g(x) \right| \\ &\le \sup_{0 \le x \le 1} |\Delta_N([0, x])| \int_0^1 \mathrm{d}|g(x)|, \end{aligned} \tag{4.48}$$

which is a form of the Koksma–Hlawka inequality [9]. The discrepancy is defined as,

$$D_N^* = \sup_{0 \le x \le 1} |\Delta_N([0, x])|$$

and $\int_0^1 \mathrm{d}|g(x)|$ is the total variation of $g(x)$. For an infinite sequence, $\lim_{N\to\infty} D_N^* = 0$ is equivalent to the sequence being uniformly distributed on I. The goal is the find a sequence of numbers such that the discrepancy is minimized and therefore, $|G_N - G|$ is minimized.

The discrepancy can be generalized to d dimensions. In this case, the set is composed of d-dimensional vectors, $\mathbf{x}_i = (x_i, x_{i+1}, \ldots, x_{i+d-1})$, occurring in a hypercubic region, $I^d = [0, 1]^d$, where $0 \le x_i \le 1$. The discrepancy is

$$\begin{aligned} D_N^* &= \sup |\Delta_N(\mathbf{x})|, \\ \Delta_N(\mathbf{x}) &= \Delta_N\left(\prod [0, \mathbf{x}_i]\right); \end{aligned} \tag{4.49}$$

where $[0, \mathbf{x}_i]$ represents a family of subintervals of I^d. D_N^* is the difference between the expected number and the actual number of vectors falling within I^d, maximized

over all such regions. A uniform deterministic grid of points has D_N^* decrease with increasing N as $O(N^{-1/d})$ in d dimensions. Improvements can be achieved and for $d \geq 2$, if the integrand $g(\mathbf{x}) = g(x_1, \ldots, x_d)$ is such that all mixed partial derivatives exist and are continuous, then sequences can be found where

$$D_N^* < C\frac{\ln^d N}{N}$$

as $N \to \infty$. The use of low-discrepancy sequences in Equation 4.47 will likely converge faster to the value of G than using pseudorandom numbers especially for regular integrands. As the dimensionality increases, the convergence rate of the q-MC calculation is dependent on the dimension d and the regularity of the integrand, while the convergence rate of the Monte Carlo calculation is guaranteed by the central limit theorem.

4.5.1 Low-Discrepancy Sequences

The characteristics of a good, low-discrepancy sequence are that it avoids clustering of points, that successive points are added so that they avoid the previously added point (a type of correlation in the structure), and that the points uniformly fill the region, I^d. A classic example of a low-discrepancy sequence is the van der Corput sequence [10] on [0, 1). For a number $n \geq 1$, n is rewritten in base b as

$$n \equiv \sum_{j=0}^{m} a_j(n) b^j, \tag{4.50}$$

where m is the integer that guarantees that $a_j(n) \equiv 0, \ \forall j > m$ and $0 \leq a_j(n) < b$. Then the number in the van der Corput sequence that corresponds to n is given by,

$$q_b(n) = \sum_{j=0}^{m} a_j(n) b^{-j-1}. \tag{4.51}$$

Consider $b = 3$, the first six integers written as in Equation 4.50 are

$$1 = 1 \times 3^0, \quad 2 = 2 \times 3^0, \quad 3 = 1 \times 3^1, \quad 4 = 1 \times 3^1 + 1 \times 3^0,$$

$$5 = 1 \times 3^1 + 2 \times 3^0, \quad 6 = 2 \times 3^1,$$

which yields the sequence,

$$q_3(1) = 1 \times 3^{-1} = \frac{1}{3}, \quad q_3(2) = 2 \times 3^{-1} = \frac{2}{3}, \quad q_3(3) = 1 \times 3^{-2} = \frac{1}{9},$$

$$q_3(4) = 1 \times 3^{-2} + 1 \times 3^{-1} = \frac{4}{9}, \quad q_3(5) = 1 \times 3^{-2} + 2 \times 3^{-1} = \frac{7}{9},$$

$$q_3(6) = 2 \times 3^{-2} = \frac{2}{9},$$

It can be shown that there exists a constant, $C(b)$, such that,

$$D_N^*(q_b(1), \ldots, q_b(N)) \leq C(b)\frac{\ln N}{N}.$$

However, the van der Corput sequence exhibits a cyclic behavior that can be problematic in many applications. Users of low-discrepancy sequences often discard the first K values and also renumber or permute the remaining values to achieve better behavior.

Most applications of q-MC involve integrals where $d > 1$, so sequences that work well in multiple dimensions are needed. The Halton sequence [11] is based on the van der Corput sequence with the first dimension derived using a base of 2. Every other dimension, s, uses a different prime base, with the bases $b_1, \ldots, b_s, \ldots$ all coprimes greater than 1. A point in d-dimensional space is chosen as,

$$\mathbf{x}_n = (q_{b_1}(n), \ldots, q_{b_d}(n)).$$

For large N, a sequence of N d-dimensional points has a discrepancy,

$$D_N(\mathbf{x}_1, \ldots, \mathbf{x}_N) \leq C(b_1, \ldots, b_d)\frac{\ln^d N}{N},$$

where $C(b_1, \ldots, b_d)$ is a constant. This sequence tends to suffer from a slower generation of new quasi-random numbers as the number of dimensions increases. Also, if N is small compared to the bases, b_s, the values of $q_{b_s}(n)$ tend to cluster near 0.

The Faure sequence [12] tries to eliminate the slowing down of the generation of multidimensional points by using just one base, b, for all dimensions. The underlying sequence is still the van der Corput sequence with the base chosen to be the smallest prime number that is greater than or equal to d, the number of dimensions in the problem. Correlation between dimensions is removed by reordering the sequence in each dimension;

$$a_i^d(n) = \sum_{j \geq i}^{m} \frac{j!}{i!(j-i)!} a_j^{d-1}(n) \ mod \ b. \tag{4.52}$$

The reordering slows down the generation of new points in all dimensions other than the first. Also, to avoid clustering of points around 0 in high dimensions, Faure recommended discarding the first $n = (b^4 - 1)$ points.

Another well-known sequence is that proposed by Sobol [13]. While it also uses the van der Corput sequence as its inspiration, a sophisticated, recursive reordering process attempts to overcome the shortcomings of previous sequences. The base, $b = 2$, is used for all dimensions and thus an initial sequence of nonnegative integers, n, $1 \leq n \leq N$, are converted into their base 2 representative, Equation 4.50. Next, for each dimension, a primitive polynomial over the Galois field of two elements is created,

$$x^s + a_1 x^{s-1} + a_2 x^{s-2} + \cdots + a_{s-1}x + 1, \tag{4.53}$$

where the a_i can be either 0 or 1. The value of s defines the degree of the polynomial. The coefficients, a_i, are used to generate odd integers, r_i, where $i = 1, \ldots, [log_2 N]$, $[y]$ indicates the smallest integer greater than y, and $0 < r_i < 2^i$,

$$r_i = 2a_1 r_{i-1} \oplus 2^2 a_2 r_{i-2} \oplus \cdots \oplus 2^d r_{i-s} \oplus r_{i-s}. \tag{4.54}$$

$\oplus$ indicates a bitwise exclusive or (addition without carry). This recursive relationship requires that r_s odd integers must be initially supplied. Once the r_i have been calculated, they are converted into a binary fraction,

$$v_i = \frac{r_i}{2^i}. \tag{4.55}$$

The conversion is accomplished by right shifting the binary expansion of r_i, Equation 4.54, by i digits. For each number, n, the rightmost 0 bit, k, is identified. The quasi-random number in the Sobol sequence [14] is then obtained as

$$q_d(n+1) = q_d(n) \oplus v_k,$$

where $q_d(0) = 0$. A primitive polynomial of a different degree, s, is used for each dimension.

The three low-discrepancy sequences described here are some of the most frequently used sequences in q-MC calculations. However, new sequences and reformulations of existing sequences continue to be introduced.

4.5.2
Error Estimation for Quasi-Monte Carlo Quadrature

Techniques to estimate the error for any asymptotic quadrature method are needed. Monte Carlo methods have the central limit theory and q-MC has the Koksma–Hlawka inequality, Equation 4.48. Unfortunately, in most cases, it is impossible to calculate error bounds based on the inequality. Also, the Koksma–Hlawka inequality is not a tight bound. That is, a q-MC integration may indeed converge even if a function has infinite variance. Much research has focused on developing easy-to-implement techniques of error estimation, and most of the techniques rely on statistical error estimation. This is achieved by applying a probabilistic structure on the low-discrepancy sets used in a calculation. One method is to scramble or permute the point sets [15]. Another uses shifted low-discrepancy sequences, which allow the central limit theorem to be applied to quasi-Monte Carlo calculations. We discuss the latter technique in more detail since it can also be viewed as a variance reduction technique for Monte Carlo calculations [16].

Let a random variable g_j be defined as,

$$g_j = \frac{1}{N} \sum_{i=1}^{N} g(\{\mathbf{x}_i + \xi_i\}), \tag{4.56}$$

where $\mathbf{x}_i$ is a vector from a low-discrepancy sequence, ξ_i is a uniform random vector in I^d and $\{\mathbf{y}\}$ indicates the vector of fractional parts of $\mathbf{y}$. The average of M independent calculations of g_j,

$$G_M = \frac{1}{M} \sum_{j=1}^{M} g_j \tag{4.57}$$

is computed and a confidence limit obtained from the central limit theorem. If $g(\mathbf{x})$ is a function with bounded variation, then the variance is found to be

$$\mathrm{var}\{g_j\} \propto O\left(\frac{\ln^{2d} N}{N^2}\right).$$

The estimator in Equation 4.56 also works for functions of infinite variance, but will have a different rate of convergence. Replacing the $\mathbf{x}_i$ with carefully chosen, ''good'' lattice points in d dimensions [9, 17] for special classes of periodic functions can reduce the variance even more.

Research continues into the important topic of error estimation in q-MC calculation [18]. It is clear that Equation 4.48 is an upper bound and studies of known integrals [19] show that actual errors can be orders of magnitude smaller than those predicted by Equation 4.48. The difficulty lies in judging the accuracy of an unknown integral in many dimensions evaluated by q-MC.

4.5.3
Applications of Quasi-Monte Carlo

The interest in and use of q-MC methods for evaluating integrals has been steadily increasing in the past several decades. The attraction is the faster rate of convergence of the numerical integration when low-discrepancy sequences are used in comparison to traditional Monte Carlo methods or other quadrature techniques. The difficulties relate to the apparent requirement of well-behaved (i.e. *smooth*) integrands and the loss of accuracy, in many cases, as the dimensionality of the problem increases.

An area where q-MC has had a substantial impact is in numerical finance where it has been used to evaluate integrals related to pricing options, financial derivatives, and the valuation of securities. Starting in the early 1990s, researchers have successfully applied q-MC to many problems and achieved convergence rates much better than the upper bound predicted by the Koksma–Hlawka inequality. Even when the high-dimensionality of the integrand suggests that q-MC may be inappropriate, hybrid methods that combine q-MC with traditional Monte Carlo have been used [20]. That is, the problem is divided such that dimensions that are smoothly varying and make a significant contribution to the integrand are evaluated using a low discrepancy sequence. All other dimensions are calculated using pseudorandom numbers and Monte Carlo with variance reduction techniques. In general, any approach that reduces the dimensionality of a problem will likely improve a q-MC calculation [21].

4.6
Comparison of Monte Carlo Integration, Quasi-Monte Carlo and Numerical Quadrature

In the introduction to this chapter, the relative efficiencies of a Monte Carlo calculation as compared with standard numerical quadrature were discussed. Several

points are worth emphasizing. For fixed expenditure of computer time, numerical quadrature is always the wiser choice in one-dimensional integration. In higher dimensions, however, the convergence of Monte Carlo integrations is independent of dimensionality, which is not true for numerical quadrature methods. Thus there is always some dimension value *d* above which Monte Carlo integrations converge faster than any fixed quadrature rule. A q-MC calculation will usually perform even better than a Monte Carlo one if the integrand is finite. The shape of the multidimensional region may be quite complicated and may make applications of a standard quadrature routine difficult. Monte Carlo methods are able to deal with essentially any finite region as are q-MC. Finally, the accuracy of a Monte Carlo estimate of an integral can always be improved by simply including some more points. In many dimensions, a fixed-point numerical quadrature rule can be improved only by going to a higher-order rule, and the previous estimate is thrown out! Error estimates for multidimensional numerical quadrature are difficult to evaluate, whereas a Monte Carlo calculation always delivers an associated error.

References

1 Kahn, M. and Marshall, A.W. (**1953**) Methods of reducing sample size in Monte Carlo computations. *Operations Research*, **1**, 263.

2 Halton, J.H. (**1965**) On the relative merits of correlated and importance sampling for Monte Carlo integration. *Proceedings of the Cambridge Philosophical Society*, **61**, 497.

3 Lavenburg, S.S. and Welch, P.D. (**1980**) A Perspective on the use of Control Variates to Increase the Efficiency of Monte Carlo. *Research Report RC8161*, IBM Corp., Yorktown Heights, New York.

4 Hammersley, J.M. and Morton, K.W. (**1956**) A new Monte Carlo technique antithetic variates. *Proceedings of the Cambridge Philosophical Society*, **52**, 449.

5 Halton, J.H. and Handscomb, D.C. (**1957**) A method for increasing the efficiency of Monte Carlo integration. *Journal of the ACM*, **4**, 329.

6 Halton, J.H. (**1980**) Generalized Antithetic Tranformations for Monte Carlo Sampling. *Computer Sciences Technical Report 408*, University of Wisconsin, Madison.

7 Karaivanova, A. and Dimov, I. (**1998**) Error analysis of an adaptive Monte Carlo method for numerical integration. *Mathematics and Computers in Simulation*, **47**, 201.

8 Kuipers, L. and Niederreiter, H. (**1974**) *Uniform Distribution of Sequences*, John Wiley & Sons, Ltd, New York.

9 Niederreiter, H. (**1978**) Quasi-Monte Carlo methods and pseudorandom numbers. *Bulletin of the American Mathematical Society*, **84**, 957.

10 van der Corput, J.G. (**1935**) Verteilungsfunktionen. I, II. *Proceedings of the Koninklijke Nederlandse Akademie Van Wetenschappen*, **38**, 813.

11 Halton, J.R. (**1960**) On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals. *Numerical Mathematics*, **2**, 84.

12 Faure, H. (**1982**) Discrépances de suites associées à un système de numération (en dimensions). *Acta Arithmetica*, **41**, 337.

13 Sobol, I.M. (**1967**) On the distribution of points in a cube and the approximate evaluation of integrals. *USSR Computational Mathematics and Mathematical Physics*, **7**, 86.

14 Bratley, P. and Fox, B.L. (**1988**) Algorithm 659: implementing Sobol's quasirandom sequence generator. *ACM Transactions on Mathematical Software*, **14**, 88.
15 Owen, A.B. (**1997**) Monte Carlo variance of scrambled net quadrature. *SIAM Journal on Numerical Analysis*, **34**, 1884.
16 Tuffin, B. (**1996**) On the use of low discrepancy sequences in Monte Carlo methods. *Monte Carlo Methods and Applications*, **2**, 295.
17 Tuffin, B. (**1998**) Variance reduction order using good lattice points in Monte Carlo methods. *Computing*, **61**, 371.
18 L'Ecuyer, P. and Lemieux, C. (**2001**) Recent advances in randomized Quasi-Monte Carlo methods, in *Modeling Uncertainty: An Examination of Stochastic Theory, Methods and Applications*, (eds M. Dror, P. L'Ecuyer and F. Szidarovszki), Kluwer, Amsterdam, pp. 607–16.
19 Schlier, Ch. (**2004**) Error trends in Quasi-Monte Carlo integration. *Computer Physics Communications*, **159**, 93.
20 Caflisch, R.E., Morokoff, W. and Owen, A. (**1997**) Valuation of mortgage-backed securities using brownian bridges to reduce effective dimension. *Journal of Computational Finance*, **1**, 27.
21 Takase, K., Moskowitz, B. and Caflisch, R.E. (**1996**) Smoothness and dimension reduction in Quasi-Monte Carlo methods. *Mathematical and Computer Modelling*, **23**, 37.

Further Reading

Berg, B.A. (**2004**) *Markov Chain Monte Carlo Simulations and their Statistical Analysis*, World Scientific, Singapore.

5
Random Walks, Integral Equations, and Variance Reduction

The term *random walk* has become almost a household term as its usage has spread from probability to the sciences and beyond, to diverse applications such as describing the behavior of the financial markets or the number of home runs hit by baseball players. What is a random walk? Let us assume that a set of random variables, $X_0, X_1, \ldots$, represent the state of a system at some "time" n for $n = 1, \ldots, N$. The probability of going from state i at time n to state j at time $n + 1$ is

$$P_{ij} = P\{X_{n+1} = j | X_n = i\}$$

and is independent of past states, prior to state i. The set $\{X_n\}$, $n \geq 0$, is called a *Markov chain* or *process* with stationary[1)] transition probabilities P_{ij}, $i, j = 1, \ldots, N$. A Markov chain is another way of referring to a random walk. The traditional example of a random walk in one dimension is of an intoxicated person moving randomly one step forward or one step backward. Another classic example is that of the "gambler's ruin." Suppose a player with a pile of money, k, plays a series of games of chance against an infinitely rich adversary. At each game, the player may win one unit of money with probability p_k and may lose one unit with probability $q_k = 1 - p_k$, $k \geq 1$. When his money is reduced to 0, the games end. The process $\{X_n\}$, where the X_n represents the amount of money remaining after n games is also a random walk.

Random walks are frequently used as discrete approximations to continuous physical processes. Consider the motion of diffusing particles, which can be described by a differential equation. The motion of the particles is continuous but the positions, subject to collisions and perhaps random forces, fluctuate randomly. If a particle's future position depends only on the current position, then the set $\{X_n\}$ where X_n is the position at a time "n" represents a Markov process.

5.1
Properties of Discrete Markov Chains

Every time the system represented by a Markov chain leaves a state i, it must be in another of the possible states; thus

1) A stationary transition probability is independent of when the transition from state i to state j occurs in the Markov chain.

Monte Carlo Methods. Second Edition. M.H. Kalos and P.A. Whitlock

ISBN: 978-3-527-40760-6

$$\sum_{j=1}^{N} P_{ij} = 1, \ i = 1, \ldots, N. \tag{5.1}$$

If state j can be reached from state i in a finite number of steps or transitions, then state j is called *accessible* from state i. If state i is accessible from state j, then the states are said to *communicate* with each other. If the two states do not communicate, then either $P_{ij} = 0$ or $P_{ji} = 0$. A Markov chain is termed *irreducible* if all states communicate with each other.

The P_{ij} form a matrix $\boldsymbol{P}$ called the *one-step transition probability matrix*. Given $\boldsymbol{P}$ and the probability distribution of the state of the process at time 0, the Markov chain is completely specified. Let P_{ij}^n be the probability that the system goes from state i to state j in n transitions. Then it can be expressed as

$$P_{ij}^n = \sum_{k=0}^{N} P_{ik}^r P_{kj}^s, \tag{5.2}$$

where $r + s = n$ and we define

$$P_{ij}^0 = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases} \tag{5.3}$$

The period of state i, $d(i)$, is the greatest common divisor of all integers $n \geq 1$ for which $P_{ii}^n > 0$. If $P_{ii}^n = 0$ for all n, then $d(i)$ is defined to be 0. If the states i and j communicate, then $d(i) = d(j)$. If all the states in a Markov chain have a period of 1, the system is called *aperiodic*.

Let f_{ii}^n be the probability that starting from state i, the first return to state i occurs at the nth transition,

$$f_{ii}^n = P\{X_n = i, X_m \neq i, m = 1, 2, \ldots, n-1 | X_0 = i\}. \tag{5.4}$$

State i is said to be *recurrent* if and only if

$$\sum_{n=1}^{N} f_{ii}^n = 1.$$

That is, starting from state i, the probability of returning to state i in finite time is 1. If this is not true, the state is said to be a *transient* state. If states i and j communicate and i is recurrent, then j is recurrent. Thus, all states in an equivalence class (i.e. states that communicate with each other) are either recurrent or transient.

Suppose we have a Markov chain with a recurrent aperiodic class of states. We can define the stationary probability for states $j = 1, 2, \ldots, N$ by

$$\pi_j = \sum_{i=0}^{N} \pi_i P_{ij}, \qquad \pi_i \geq 0,$$

$$\sum_{i=0}^{N} \pi_i = 1. \tag{5.5}$$

π_j is the proportion of the time that the system spends in state j. The quantity $\pi_i P_{ij}$ is the proportion of the time that the random walk has just entered state j from state i. If the initial state of the random walk is chosen to be distributed as π_j, then $P\{X_n = j\}$ is equal to π_j, for all n and j.

If $\pi_i > 0$ for one state i in an aperiodic recurrent class, then $\pi_j > 0$ for all states j in the same class. Such a class is called *strongly ergodic*. When

$$\pi_i P_{ij} = \pi_j P_{ji} \tag{5.6}$$

for all $i \neq j$, then the Markov chain is said to be *time reversible*. If the initial state X_0 is chosen from the set $\{\pi_j\}$, the sequence of steps going backwards in time from any point n will also be a Markov chain with transition probabilities given by P_{ij}.

5.1.1 Estimators and Markov Processes

Markov chains are used in simulations to model the behavior of systems whose probability distribution functions are not easily sampled. Suppose that a discrete random variable has a probability mass function given by $p_j = P\{X = j\}$, $j = 1, 2, \ldots, N$. It can be sampled by creating an irreducible aperiodic Markov chain such that $p_j = \pi_j$ for $j = 1, 2, \ldots, N$ and obtaining the values of X_n when n is large. An estimator for a property, $h(X)$, of the system, $E(h(X)) = \sum_{j=1}^{N} h(j)p_j$ can be formed from the states reached in the random walk,

$$E(h(X)) \approx \frac{1}{m} \sum_{i=1}^{m} h(X_i). \tag{5.7}$$

However, at step n in a Markov chain, the state of the next step, $n + 1$, is dependent on the properties of the previous step. Thus, it takes some number of steps, not always easily quantified, to lose the influence of the distribution of the initial state X_0. As a result, in forming estimators of quantities of interest, the first k steps of the Markov chain are usually discarded. The estimator for the property $h(X)$ then becomes,

$$E(h(X)) \approx \frac{1}{m-k} \sum_{i=k+1}^{m} h(X_i). \tag{5.8}$$

The choice of k is guided by the properties of the application.

The strong serial correlation that exists between the steps of a Markov chain also effect the estimation of the standard error of the estimator in Equation 5.8. To correct for the correlation, one approach is to divide the Markov chain into blocks large enough so that the correlation is minimized between the blocks. This approach is called *batch means* or *blocking*. The $m - k$ steps in Equation 5.8 are broken up into s blocks or batches of length r steps, where $s = \frac{m-k}{r}$ and both s and r are integers. The average value of $h(X)$ is evaluated for each of the s blocks,

$$H_\ell = \frac{1}{r} \sum_{i=k+(\ell-1)r+1}^{k+\ell r} h(X_i), \quad \ell = 1, 2, \ldots, s. \tag{5.9}$$

Since each of the H_ℓ is considered to be an independent and identically distributed random variable, the mean value is given by

$$\overline{H} = \frac{1}{s} \sum_{\ell=1}^{s} H_\ell \tag{5.10}$$

and $\overline{H}$ is used to obtain the sample estimate of the variance,

$$\mathrm{var}\{H_\ell\} = \frac{1}{s-1} \sum_{\ell=1}^{s} (H_\ell - \overline{H})^2. \tag{5.11}$$

The estimate of the standard error associated with $E(h(X))$ can then be obtained as $\sqrt{\mathrm{var}\{H_\ell\}/s}$.

5.2 Applications Using Markov Chains

One method based on Markov chains has already been discussed, the M(RT)^2 method introduced in Section 3.7. There, the probability for observing an equilibrium system, independent of time, near a random variable X was $f(X)$. X represents the state of the system, i.e. the coordinates of all the particles in the system. A slight change in notation would describe the M(RT)^2 algorithm as sampling the sequence of states, $X_0, X_1, \ldots, X_i, \ldots$. The probability for observing a system near X_i, $f(X_i)$, corresponds to π_i in Equation 5.5. The kinetics of the system must obey detailed balance, Equation 3.89,

$$K(X_i|X_j) f(X_j) = K(X_j|X_i) f(X_i). \tag{5.12}$$

Equating $K(X_i|X_j)$ with P_{ij}, Equation 5.12 is equivalent to Equation 5.6. Using this equivalence, the Markov chain representing the M(RT)^2 random walk is given by[2)]

$$\begin{aligned} P_{ij} &= K(X_i|X_j) = A(X_i|X_j) T(X_i|X_j), \quad \text{for } j \neq i, \\ P_{ii} &= K(X_i|X_i) = T(X_i|X_i) + \sum_{k \neq i} (1 - A(X_i|X_k) T(X_i|X_k)). \end{aligned} \tag{5.13}$$

P_{ii} is the probability that the Markov chain stays at the same state of the system, X_i. The Markov chain that results from the M(RT)^2 algorithm is an ergodic, irreducible, reversible random walk.

2) This representation of the algorithm assumes the $\{X_n\}$ are a large but finite number of states.

5.2.1 Simulated Annealing

Kirkpatrick *et al.* [1] introduced the simulated annealing method, a generalization of ideas embedded in the M(RT)^2 algorithm, to address combinatorial optimization problems. Their initial application was to obtain an optimized wiring pattern between integrated circuits on a circuit board, which is similar to the classic traveling salesman problem. In the latter problem, a salesman must visit n cities and wishes to travel the shortest distance without returning to any city. A path is a sequence of cities labeled by the natural numbers, $X = \{x_1, x_5, x_2, \ldots\}$, contained in the set of all permutations of $\{x_1, \ldots, x_n\}$. However, some of the paths are forbidden. If $\mathrm{d}(x_{i-1}, x_i)$ is the distance between city i and $i-1$, the total distance or cost is

$$U(X) = \sum_{i=2}^{n} \mathrm{d}(x_{i-1}, x_i),$$

with forbidden paths having an infinite cost. The probability distribution of the paths can be assigned as

$$F(X) = \text{const}\, \mathrm{e}^{-\lambda U(X)}. \tag{5.14}$$

As λ becomes large, only the optimal paths will have finite probability.

Recognizing the similarity between X and the Gibb's measure,

$$F(X) \propto \exp\left(\frac{1}{kT} U(X)\right). \tag{5.15}$$

Kirkpatrick *et al.* proposed letting $\lambda \propto \frac{1}{kT}$. A path X would be selected using the M(RT)^2 algorithm for a fixed value of λ. The parameter would be initially small (high temperature) and the equilibrium probability distribution of paths would be quickly achieved. Then λ is increased slowly (annealing) to allow the equilibrium distribution of paths to be selected at each value of λ. Eventually, at large enough λ, only the optimal paths would survive.

In the Markov chain terminology, let $\{X_n\}$ be a finite set of states and let $U(X)$ be a nonnegative function of the $\{X_n\}$. The goal is to find the maximum (or minimum) value of $U(X)$ and at least one state, M, corresponding to it,

$$U^* = \max_{\{X_n\}} U(X)$$

and

$$M = \{X \in \{X_n\} : U(X) = U^*\}.$$

The probability mass function for the X_i is given by

$$p(X) = \frac{\mathrm{e}^{\lambda U(X)}}{\sum_{\{X_n\}} \mathrm{e}^{\lambda U(X)}}, \tag{5.16}$$

where λ is assumed to be greater than 0. Multiplying both the numerator and the denominator by $\exp(-\lambda U^*)$, Equation 5.16 becomes

$$p(X) = \frac{e^{\lambda(U(X)-U^*)}}{\sum_{\{X_n\}} e^{\lambda(U(X)-U^*)}}. \tag{5.17}$$

However, when $U(X) = U^*$, the contribution to the sum in the denominator is 1 and Equation 5.17 may be rewritten as

$$p(X) = \frac{e^{\lambda(U(X)-U^*)}}{|M| + \sum_{X \notin M} e^{\lambda(U(X)-U^*)}}, \tag{5.18}$$

where $|M|$ indicates the number of states with $U(X) = U^*$. The quantity $U(X) - U^*$ is always less than or equal to 0. So as $\lambda \to \infty$,

$$p(X) \to \frac{\delta(X)}{|M|},$$

where $\delta(X) = 1$ if $U(X) = U^*$ and 0, otherwise.

In practice, some schedule must be used to change the value of λ at each step in the annealing process to guarantee convergence. If the annealing is assumed to occur in m steps, then one possibility is to let $\lambda_m = \text{const} \times \log(1 + m)$, where const > 0. The value of $U(X)$ is monitored and when a maximum value is reached for large λ_m, this value of X is considered to be in the set M.

The advantage of using the M(RT)^2 algorithm to sample the states $\{X_n\}$ is that the local maxima or minima can be avoided. The transition probability from one state X_j to another X_i, $T(X_i|X_j)$, is of course dependent on the application. In the traveling salesman problem, X_i may be a different permutation of the order of cities visited. If X_i is a forbidden case, $p(X)$ will be 0. With probability

$$A(X_i|X_j) = \min\left\{1, \frac{\exp(\lambda_n U(X_i) T(X_i|X_j))}{\exp(\lambda_n U(X_j) T(X_j|X_i))}\right\}, \tag{5.19}$$

the new state is accepted; otherwise, the system stays in the current state. Thus, there is always a probability of leaving a local maxima for another state, even one that is less favorable.

Simulated annealing is widely used for optimization in many diverse fields. A thorough discussion of the method and typical applications is given in van Laarhoven and Aarts [2].

5.2.2 Genetic Algorithms

Another random walk technique that is used to search complex spaces, genetic algorithm (GAs), was inspired by population genetics [3]. In this method, a search over many generations is propagated by evaluating the fitness of individuals in a gene pool. Individuals for the next generation are selected by operating on

individuals in the current generation and the process is iterated until the system ceases to improve as measured by some fitness criteria.

Most applications of GAs use either fixed length binary strings or multidimensional grids to represent prospective solutions to a problem. Each position in the string represents a particular feature of interest and the bits are usually assumed to not interact. The individual strings compose a population that evolves from generation to generation, becoming more ''fit,'' i.e. approaching the correct solution, as the random walk continues. A next generation is produced by several possible events. The crossover event occurs when two strings (parents) are selected, either randomly or on the basis of their fitness, and substrings are swapped. Whether a crossover event is chosen is governed by a probability. The decision to accept the new strings into the next generation may be based on whether they are more fit than their parents or other individuals, or may be decided randomly. Strings not involved in crossover may be cloned for the next generation based on their fitness. With a small probability, mutation, that is, flipping one or more bits of an individual, can also occur. Mutation allows new information to be introduced into the prospective solutions and also reduces the likelihood that the system will be stuck in a local minima or maxima. The probability of mutation should be small or the evolutionary nature of the algorithm will be lost.

A phenomenological description of the method is as follows:

1. Start with a randomly selected population representing a set of solutions, e.g. a bit string γ, to the problem of interest.
2. Evaluate the fitness of each string by applying an objective function, $f(\gamma)$.
3. Produce the next generation of strings by iterating the following steps until the population is complete:
   - Either randomly or on the basis of fitness, select two parents.
   - With the crossover probability, swap randomly selected subsequences in the two parents.
   - If crossover is not selected, the offspring are identical to the parents.
   - With the mutation probability, flip one or more bits of a selected offspring.
   - Replace two strings in the next generation, either the parents, randomly selected strings, or strings based on fitness criteria.
4. Decide whether the ending condition has been satisfied. If it has, stop and return the best solution based on the objective function.
5. Otherwise, return to step 2.

If the initial population size is too small, the simulation will take a long time to converge. A very large population size will not improve the rate of convergence and increases the time spent in generating a new population. The bit strings or grids can represent numbers or each bit can indicate that a particular, fixed function

is turned on or off. A string may also represent a permutation. GAs have found wide applications in structural design [4], routing problems [5], optimization [6], machine learning [7], and biological studies [8].

Nix and Vose [9] developed a mathematical framework that showed that simple GAs can be modeled with Markov chains. In their formulation, the states of the Markov chain are the populations of solutions, fixed-length binary strings, in each generation. It allows one point crossovers to occur and proportional selection of strings. The transition probabilities from one state to the next are obtained from a multinomial probability distribution. Let X and Y correspond to the populations of two succeeding generations. The transition probability from Y to X is given by

$$T(X|Y) = r! \prod_{j \in \Omega} \frac{\mathcal{G}(Y/r)_j^{X_j}}{X_j!}, \tag{5.20}$$

where Ω represents the sample space of ordered strings of length ℓ and the number of possible strings is $r = 2^\ell$. $\mathcal{G}(Y/r)_j$ is the probability, given the current population is Y/r, that a sequence, j, is added to the next generation. The probability that sequence j is in X is $\prod \mathcal{G}(Y/r)_j^{X_j}$. The number of sequences corresponding to population X is $r!/\prod X_j!$.

Vose [10] generalized the model to describe a ''random heuristic search,'' where each solution in the next generation is selected independently from the current generation. Research continues to show how Markov chains model steady-state algorithms and more general selection techniques [11].

5.2.3
Poisson Processes and Continuous Time Markov Chains

The discussion below analyzes the properties of Poisson processes as Markov chains. However, another approach labeled *discrete event simulation* models an inherently stochastic system by generating artificial random events on a computer. There are several characteristics that are necessary for a well-designed simulation. A clear statement of the system to be simulated is needed. Once this is accomplished, the probability distribution functions that will be sampled must be identified and explicitly defined. Then methods are developed to sample all the required pdf's. And finally, the resulting statistics from the events must be analyzed to draw conclusions about the system. Such simulations are widely applicable to many fields; for example, a computer operating system may be tested by giving it a randomly generated operating environment [12]. Areas of physics in which discrete event simulations are often employed are radiation transport [13], heat transfer [14], and nuclear theory [15]. Reliability theory [16] is another important area of application; as are queuing theory [17] and financial simulations [18]. A description of the discrete event approach is more fully developed in the discussion of radiation transport in Sections 6.1 through 6.4. For a more general description, see Ross [19] or Law and Kelton [20].

The previous examples of Markov processes assumed that the events were independent of actual time. However, that assumption excludes many physical systems. In a Poisson process, time is considered to be continuous, $t = [0, \infty)$, and the random variable $X(t)$ counts the number of occurrences of a specific event between times 0 to t. One concrete example of such a process is the number of X rays emitted during radioactive decay if the period of observation is much less than the half-life of the radioactive element. Another well-known example is the arrival of customers to a queue.

A Poisson process is defined by the following properties:

1. The number of events happening in two different time intervals are independent.
2. $X(t_0 + t) - X(t_0)$ depends only on t and not on t_0 or $X(t_0)$.
3. Two or more events do not occur simultaneously.

The probability of at least one event happening in a time $h \to 0$ is

$$p(h) = \alpha h + g(h), \tag{5.21}$$

where $\alpha > 0$. What is the probability, $F_m(t) = P\{X(t) = m\}$, of exactly m events occurring in the time interval 0 to t? From property 1 above, the probability of no events occurring in the time period $t + h$ is given by

$$F_0(t + h) = F_0(t) \times F_0(h)$$

and using the fact that no events at time h is given by $(1 - p(h))$,

$$F_0(t + h) = F_0(t)(1 - p(h)).$$

Subtracting $F_0(t)$ from each side and dividing by h yields

$$\frac{\mathrm{d}F_0(t)}{\mathrm{d}t} = \frac{F_0(t + h) - F_0(t)}{h} = -F_0(t)\frac{p(h)}{h}.$$

Using Equation 5.21,

$$\lim_{h \to 0} \frac{p(h)}{h} \to \alpha$$

gives

$$\frac{\mathrm{d}F_0(t)}{\mathrm{d}t} = -\alpha F_0(t) \quad \text{or} \quad F_0(t) = \text{const}\, \mathrm{e}^{-\alpha t}. \tag{5.22}$$

If the initial condition is that $F_0(0) = 1$, then the constant in Equation 5.22 is 1 and the probability of exactly no events at time t is

$$F_0(t) = \mathrm{e}^{-\alpha t}. \tag{5.23}$$

Following a similar analysis for each value of m, it can be shown that

$$F_m(t) = \frac{\alpha^m t^m}{m!} e^{-\alpha t}. \tag{5.24}$$

Thus, $X(t)$ follows a Poisson distribution with parameter αt (see Section 2.2.3).

The Poisson process is an example of a continuous time Markov process with stationary transition probabilities. That is, for $t > 0$,

$$P_{ij}(t) = P\{X(t+u) = j | X(u) = i\}; \quad i, j = 0, 1, \ldots; \tag{5.25}$$

and the $P_{ij}(t)$ are independent of $u > 0$. Other properties of the Markov chain representing a Poisson process are

1. $P_{ij}(t) \geq 0, \quad t > 0;$
2. $\sum_j P_{ij}(t) = 1, \quad t > 0;$
3. $\sum_k P_{ik}(t) P_{kj}(h) = P_{ij}(t+h), \quad t \text{ and } h > 0;$
4. $\lim_{t \to 0} P_{ij}(t) = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}.$

The properties in 1–4 above imply that $P_{ij}(t)$ is differentiable for every $t \geq 0$.

Birth Processes

The systems that Poisson processes model can be extended if one or more of the assumptions listed prior to Equation 5.21 is relaxed. In a pure birth process, the chance of an event occurring at time t is dependent on the number of events which have already occurred. This is a relaxation of the assumption that events happening in two different time intervals are independent. An example of a birth process is the growth of a population of bacteria in a favorable environment with no mortality or migration. The probability of producing new bacteria at any time t is directly proportional to the population size.

Let $X(t)$ denote the number of births in the time interval $[0, t]$ with the initial condition that $X(0) = 0$. A birth process also describes a Markov process with

$$\begin{aligned} P_{i,j}(h) &= P\{X(t+h) - X(t) = 1 | X(t) = i\} = \lambda_i h + g_{1,i}(h), \quad j = i + 1, \\ P_{i,i}(h) &= P\{X(t+h) - X(t) = 0 | X(t) = i\} = 1 - \lambda_i h + g_{0,i}(h). \end{aligned} \tag{5.26}$$

Let the probability that exactly m births have occurred by time t,

$$F_m(t) = P\{X(t) = m\},$$

then it can be shown using Equation 5.26 that

$$\frac{dF_0(t)}{dt} = -\lambda_0 F_0(t), \tag{5.27a}$$

$$\frac{dF_m(t)}{dt} = -\lambda_m F_m(t) + \lambda_{m-1} F_{m-1}(t), \quad m \geq 1. \tag{5.27b}$$

With the initial condition that $F_0(0) = 1$, Equation 5.27a can be solved to yield

$$F_0(t) = e^{\lambda_0 t}.$$

If all the $\lambda_m \geq 0$ and the initial conditions are $F_m(0) = 0$ for $m > 0$, then Equation 5.27b can be integrated to obtain

$$F_m(t) = \lambda_{m-1} e^{-\lambda_m t} \int_0^t e^{\lambda_m u} F_{m-1}(u)\, du. \tag{5.28}$$

Returning to the example of multiplying bacteria, let there be one bacterium present at $t = 0$. Assume that the probability of a bacterium splitting into two in a time interval h is

$$p(h) = \alpha h + g(h), \quad \alpha > 0,$$

and that each bacterium is independent and does not interact with any other bacteria. Then, using the binomial theorem,

$$\begin{aligned} P\{X(t+h) - X(t) = 1 | X(t) = m\} &= \binom{m+1}{1} (\alpha h + g(h))(1 - \alpha h + g(h))^m \\ &= (m+1)\alpha h + g_m(h). \end{aligned}$$

Comparing with Equation 5.26, $\lambda_m = (m+1)\alpha$ and

$$\frac{dF_m(t)}{dt} = -\alpha((m+1)F_m(t) - mF_{m-1}(t)), \quad m = 0, 1, \ldots, \tag{5.29}$$

with initial conditions $F_0(0) = 1$ and $F_m(0) = 0$, for $m > 0$. Equation 5.29 may be integrated to find the probability that exactly m new bacteria are produced at time t,

$$F_m(t) = e^{-\alpha t}(1 - e^{-\alpha t})^m, \quad m \geq 0. \tag{5.30}$$

The time between consecutive dividings of the bacteria is exponentially distributed with parameter $(m+1)\alpha$.

Birth/Death Processes

The population of a system can decrease as well as increase with time. For example, the number of bacteria in a culture changes with time through death and migration, as well as the splitting of individual bacterium. Or a population can change through mutation, as well as through splitting. These systems are described as birth/death processes and are also examples of a Markov process with stationary transition probabilities,

$$P_{ij}(t) = P\{X(t+u) = j | X(u) = i\}.$$

All the $P_{ij} \geq 0$ and as before, $\sum_{j=0}^{\infty} P_{ij}(t) = 1$. However, now there are both rates of births, λ_i, and rates of deaths, μ_i. Let $\mu_0 = 0$ and $\lambda_0 = 0$ with μ_i, $\lambda_i > 0$ for

$i = 1, 2, \ldots$, then the transition probabilities for small time, $h \to 0$, are given by

$$\begin{aligned} P_{ij}(h) &= \lambda_i h + g_{1,i}(h), \quad j = i + 1, \\ P_{ii}(h) &= 1 - (\lambda_i + \mu_i)h + g_{0,i}(h), \\ P_{ij}(h) &= \mu_i + g_{-1,i}(h), \quad i \geq 0,\ j = i - 1. \end{aligned} \tag{5.31}$$

Since the process is Markovian,

$$P_{ij}(t + u) = \sum_{k=0}^{\infty} P_{ik}(t) P_{kj}(u). \tag{5.32}$$

To determine the probability that the system is in state m,

$$F_m(t) = P\{X(t) = m\}, \tag{5.33}$$

we need to know the probability distribution of the initial state. Let $I_i = P\{X(0) = i\}$ be the probability of being in state i at $t = 0$, then

$$F_m(t) = \sum_{i=0}^{\infty} I_i P_{im}(t). \tag{5.34}$$

Using Equation 5.34, it can be shown that the amount of time, T_j, that the system stays in state j is distributed exponentially:

$$\begin{aligned} W_j(t) &= P\{T_j \geq t\}, \\ W_j(t) &= \mathrm{e}^{-(\lambda_j + \mu_j)t}. \end{aligned} \tag{5.35}$$

To simulate a birth/death process, the parameters λ_i and μ_i need to be assigned for all the possible states in the system. Let the system begin in state i and remain there for a period of time t_1. This time, t_1, is sampled from the exponential function given by Equation 5.35. The decision to move to states $i + 1$ or $i - 1$ is governed by the probabilities $p_i = \lambda_i/(\lambda_i + \mu_i)$ and $(1 - p_i) = \mu_i/(\lambda_i + \mu_i)$, respectively. The sampling of the time interval in the next state, $i \pm 1$, is again done from Equation 5.35. A chain of states or realization is simulated until the elapsed time is large or the system is no longer of interest. One possible path is given in Table 5.1. A set of these paths represents the $P_{ij}(t)$ given by Equations 5.31.

An example of a birth/death process is given by a collection of N spin particles, where each particle can either be spin *up* or spin *down*. The conversion from one spin to the other is spontaneous and a change from an *up* spin to a *down* spin can be considered a death of the *up* spin. Let $X(t)$ represent the number of *up* spins at time t,

$$X(t) = i, \quad 0 \leq i \leq N.$$

The probability that the population changes in the time interval $(t, t + h)$ is

$$p(h) = \alpha h + g(h),$$

Table 5.1 A part of a chain of states or realization for a birth/death process.

State, $X(t)$	Time interval
i	$0 < t < t_1$
$i-1$	$t_1 < t < t_1 + t_2$
$i-2$	$t_1 + t_2 < t < t_1 + t_2 + t_3$
$i-1$	$t_1 + t_2 + t_3 < t < t_1 + t_2 + t_3 + t_4$
$\vdots$	$\vdots$

where $\alpha > 0$. If a change in state occurs, i.e. the population of *up* spins changes, then several events must occur. The probability that an *up* spin is selected is i/N and the probability that it is converted to a *down* spin is β_1. The probability that a *down* spin is chosen is $1 - i/N$ and the probability that it changes to an *up* spin is given by β_2. So, for the selected spin to result in an *up* spin one of two possible scenarios must occur:

1. The spin was an *up* spin and no change occurred with probability $\frac{i}{N}(1-\beta_1)$.
2. The spin was a *down* spin and was converted with probability $(1 - i/N)\beta_2$.

The conditional probability that at time $(t+h)$ the population of *up* spins has increased by 1 given that $X(t) = i$ is

$$\left(1 - \frac{i}{N}\right)\left(\frac{i}{N}(1-\beta_1) + \left(1 - \frac{i}{N}\right)\beta_2\right),$$

since an increase in *up* spins means the death of *down* spins. Likewise, the conditional probability that at time $t+h$ the population of *up* spins has decreased by 1 given that $X(t) = i$ is

$$\frac{i}{N}\left(\left(1 - \frac{i}{N}\right)(1-\beta_2) + \frac{i}{N}\beta_1\right),$$

since an *up* spin had to die.

The birth/death process has a finite number of states, $0 \le i \le N$ and at each change of state i, the birth rate is given by

$$\lambda_i = \alpha\left(1 - \frac{i}{N}\right)\left(\frac{i}{N}(1-\beta_1) + \left(1 - \frac{i}{N}\right)\beta_2\right),$$

and the death rate is given by

$$\mu_i = \alpha\frac{i}{N}\left(\frac{i}{N}\beta_1 + \left(1 - \frac{i}{N}\right)(1-\beta_2)\right).$$

An alternative method of modeling spin systems is described in Chapter 7.

The transition probabilities for birth/death processes are described by a system of differential equations called *the backward Kolmogorov differential equations*:

$$\frac{P_{0j}(t)}{dt} = -\lambda_0 P_{0j}(t) + \lambda_0 P_{1j}(t),$$
$$\frac{P_{ij}(t)}{dt} = \mu_i P_{(i-1)j}(t) - (\lambda_i + \mu_i) P_{ij}(t) + \lambda_i P_{(i+1)j}(t), \quad i \geq 1, \tag{5.36}$$

with $P_{ij}(0) = \delta_{ij}$. These equations may be derived using Equations 5.31 and 5.32 and by decomposing a time interval $(0, t+h)$ into two time intervals $(0, h)$ and $(h, t+h)$. Then each of the new time intervals are analyzed separately. Alternatively, the forward Kolmogorov differential equations can be derived by considering a time interval $(0, t+h)$ divided into periods $(0, t)$ and $(t, t+h)$. Such an analysis yields,

$$\frac{P_{i0}(t)}{dt} = -\lambda_0 P_{i0}(t) + \mu_1 P_{i1}(t), \tag{5.37}$$
$$\frac{P_{ij}(t)}{dt} = \lambda_{j-1} P_{i(j-1)}(t) - (\lambda_j + \mu_j) P_{ij}(t) + \mu_{j+1} P_{i(j+1)}(t), \quad j \geq 1.$$

However, a birth/death process can be simulated without ever deriving and solving either Equation 5.36 or 5.37. As described above, an event, birth or death, is chosen from the appropriate distribution function. The time interval of each new random event can be sampled from the appropriate exponential distribution and the system moved forward by this time to create one step in a realization of a Markov chain of events.

Absorbing States

The birth/death process can be further generalized by allowing a constant rate of migration in or out of the system in addition to birth and death. Another very important generalization is that of an absorbing state or states. An absorbing state is one in which $\lambda_m = 0$ or once entered, the state m can never be left and the Markov process ends.

An example of such a process is when a closed system, for example, a bacteria culture, has only growth and death without any external intervention. If the population reaches 0, the culture is dead. This is not a certain outcome, since, depending on the rates of each event, the system may wander forever among the nonabsorbing states.

To analyze the likelihood of eventual absorption, consider a system where λ_i is the birth rate for state i and μ_i is the death rate. Let A_i be the probability of absorption into state 0, the absorbing state, from state i, where $i \geq 1$ and $0 \leq A_i \leq 1$. As discussed previously, a change of state to $i+1$ occurs with probability $\lambda_i/(\mu_i + \lambda_i)$ or it changes to $i-1$ with probability $\mu_i/(\mu_i + \lambda_i)$. If it is assumed that $A_0 = 1$, i.e. once state $i = 0$ is reached it is not left, a recursion for A_i can be developed:

$$A_i = \frac{\lambda_i}{(\mu_i + \lambda_i)} A_{i+1} + \frac{\mu_i}{(\mu_i + \lambda_i)} A_{i-1}. \tag{5.38}$$

Rewriting Equation 5.38 as

$$A_{i+1} - A_i = \frac{\mu_i}{\lambda_i}(A_i - A_{i-1}), \tag{5.39}$$

it can be iterated starting at $j = 1$ to obtain all the contributions from previous states to $j = i$. Summing all the states from $i = 1$ to $i = m$ yields

$$A_{i+1} - A_1 = (A_1 - 1)\sum_{i=1}^{m}\left(\prod_{j=1}^{i}\frac{\mu_j}{\lambda_j}\right), \tag{5.40}$$

where $m \geq 1$. If we assume that $0 \leq A_1 \leq 1$, then the summation on the right-hand side of Equation 5.40 must be less than infinity and A_m is decreasing and approaches 0 as $m \to \infty$. Letting $m \to \infty$, Equation 5.40 can be solved for A_1:

$$A_1 = \frac{\displaystyle\sum_{i=1}^{\infty}\left(\prod_{j=1}^{i}\mu_j/\lambda_j\right)}{1 + \displaystyle\sum_{i=1}^{\infty}\left(\prod_{j=1}^{i}\mu_j/\lambda_j\right)}. \tag{5.41}$$

Using this result, the probability for absorption into state 0 from state $m + 1$, $m \geq 1$ is

$$A_{m+1} = \frac{\displaystyle\sum_{i=m+1}^{\infty}\left(\prod_{j=1}^{i}\mu_j/\lambda_j\right)}{1 + \displaystyle\sum_{i=1}^{\infty}\left(\prod_{j=1}^{i}\mu_j/\lambda_j\right)}. \tag{5.42}$$

We can also calculate the mean time to absorption using Equation 5.35. Since the waiting time that the system spends in each state i is exponentially distributed, the mean waiting time is given by $(\mu_i + \lambda_i)^{-1}$. A recursion relationship can be developed for w_i, the mean absorption time starting from state i,

$$w_i = \frac{1}{\mu_i + \lambda_i} + \frac{\lambda_i}{\mu_i + \lambda_i}w_{i+1} + \frac{\mu_i}{\mu_i + \lambda_i}w_{i-1}. \tag{5.43}$$

Similar to the analysis above, Equation 5.43 is rewritten as

$$w_i - w_{i+1} = \frac{1}{\lambda_i} + \frac{\mu_i}{\lambda_i}(w_{i-1} - w_i),$$

and then iterated and summed over all states. Eventually, it can be shown that the mean time to absorption from state 1 is

$$w_1 = \sum_{i=1}^{\infty}\frac{1}{\mu_i}\prod_{k=1}^{i-1}\frac{\lambda_k}{\mu_k}. \tag{5.44}$$

As an example of a birth/death process with an absorbing state, consider an isolated bacteria culture. The culture exhibits a linear growth in population proportional to its size, $\lambda_m = m\alpha$, and is balanced by a linear decrease in size, $\mu_m = m\beta$, due to death. The probability that the population size at time t is m is given by

$$F_m(t) = P\{X(t) = m\},$$

with the initial condition that at $t = 0$, $X(t) = i$. However, depending on the values of α and β, the culture can die out, $X(t) = 0$. The probability of absorption from any state can be calculated from Equation 5.42 for $m \geq 1$:

$$A_m = \begin{cases} \left(\dfrac{\beta}{\alpha}\right)^n & \beta < \alpha \\ 1 & \beta \geq \alpha. \end{cases}$$

If $\beta > \alpha$, the mean time until absorption from state $m = 1$ can be calculated from Equation 5.44,

$$w_1 = \sum_{i=1}^{\infty} \frac{1}{i} \left(\frac{\alpha}{\beta}\right)^{i-1},$$

which can be reduced to

$$w_1 = -\frac{\beta}{\alpha} \log\left(1 - \frac{\alpha}{\beta}\right).$$

5.2.4 Brownian Motion

In the early nineteenth century, an English botanist, Mr Brown, published his observation that small particles floating in still water moved ceaselessly in an erratic pattern. Later, Einstein postulated that the particles were colliding with the water or solvent molecules and derived a mathematical description based on physical laws.

In one dimension, let $X(t)$ represent the position (x coordinate) of a particle at time t. The quantity $p(x, t|x')$ represents the conditional probability that $X(t + t') = x$ given that $X(t') = x'$ and that the transition is stationary in time. The conditional probability satisfies

$$p(x, t|x') \geq 0 \quad \text{and} \quad \int_{-\infty}^{\infty} p(x, t|x')\, dx = 1.$$

Furthermore, as $t \to 0$, the new position of the particle, x, is likely to be near the previous position, x',

$$\lim_{t \to 0} p(x, t|x') = 0, \quad \text{for } x \neq x'.$$

Physically, the conditional probability must satisfy the differential equation

$$\frac{\partial p(x,t|x')}{\partial t} = D\frac{\partial^2 p(x,t|x')}{\partial x^2}, \tag{5.45}$$

where D is the diffusion constant. This equation can be solved directly to yield

$$p(x,t|x') = \sqrt{\tfrac{D}{\pi t}}\mathrm{e}^{-D(x-x')^2/t}. \tag{5.46}$$

However, Brownian motion can also be considered as an example of a continuous time, continuous state space Markov process. This can be modeled as a discrete random walk where the steps in the random walk represent the time increments. Let the particles move on a lattice in one dimension and $p_j(m)$ be the probability that a particle is j lattice points to the right ($j > 0$) of its initial position at time m. Assuming that a move to the right or left is equally likely, a recursion for $p_j(m)$ may be derived:

$$p_j(m+1) = \tfrac{1}{2}p_{j+1}(m) + \tfrac{1}{2}p_{j-1}(m).$$

This can be rewritten by subtracting $p_j(m)$ from each side to give

$$p_j(m+1) - p_j(m) = \tfrac{1}{2}(p_{j+1}(m) - 2p_j(m) + p_{j-1}(m)). \tag{5.47}$$

If the time between transitions, δ, and the size of the steps, h, are allowed to decrease toward 0 such that $\delta = h^2$, Equation 5.47 becomes

$$\frac{p_{jh}((m+1)\delta) - p_{jh}(m\delta)}{\delta} = \frac{\frac{1}{2}(p_{(j+1)h}(m\delta) - 2p_{jh}(m\delta) + p_{(j-1)h}(m\delta))}{\delta},$$

which is the discrete analog of Equation 5.45. Thus, as in the case of Poisson processes, a discrete random walk can be used to represent the solution to a differential equation.

The properties of Brownian motion can be summarized as follows:

1. The change in position $X(t+t') - X(t')$ is distributed as a Gaussian with a mean of zero and a variance given by D/t.
2. For any pair of disjoint time intervals, $[t_1, t_2]$ and $[t_3, t_4]$, the changes in position, $X(t_2) - X(t_1)$ and $X(t_4) - X(t_3)$, are independent random variables distributed as in 1.

The discrete random walk in one dimension is defined by assigning the probabilities of a move to the right, to the left, and for staying in place. For classic Brownian motion, the probability of moving in either direction is $\frac{1}{2}$ and for staying in place is 0. The random walk can be modified by changing the probabilities and by restricting the states (positions) that can be visited. For example, the states can be restricted to the nonnegative integers and by giving the zero state a special meaning. If the probability of moving to the zero state is $p_0(m) = 1$, then the zero state is a reflecting barrier. A move to zero is always followed by a move to state 1. If $p_0 = 0$, a move to the zero state means absorption and the random walk ends.

If $0 < p_0(m) < 1$ and the probability of staying in place is nonzero, the zero state becomes a partially reflecting boundary. Other states can have similar behavior as well.

Of course, Brownian motion occurs in more than one dimension. A straightforward generalization to n dimensions is possible. Consider a set of integral lattice points in n-dimensional Euclidean space. A point is represented by $\boldsymbol{k} = (k_1, \ldots, k_n)$. The random walk develops by moves to a nearest neighbor with the transition probability given by

$$P_{\boldsymbol{k}\boldsymbol{\ell}} = \begin{cases} \dfrac{1}{2n} & \sum_{i=1}^{n} |\ell_i - k_i| = 1 \\ 0 & \text{otherwise.} \end{cases} \tag{5.48}$$

5.3 Integral Equations

The discussions up to now have shown that random walks can represent various systems whose behavior is described by differential equations; i.e. Brownian motion and the diffusion equation or generalized Poisson processes, and the forward and backward Kolmogorov differential equations. However, there are some very important problems that are most properly described by integral equations such as transport phenomena; we shall develop random walk techniques that will allow their solution using Monte Carlo methods as well. Indeed, we shall be motivated to reformulate problems into integral equations so as to be able to exploit the use of random walks.

5.3.1 Radiation Transport and Random Walks

To clarify the relationship between a random walk and an integral equation, let us outline in the sparsest possible way the steps needed to perform a Monte Carlo simulation of radiation transport.

1. Formulate a description of the sources of radiation. Interpret that description as a probability distribution function. Sample the probability distribution function to specify initial values of the coordinates in the simulation.
2. Formulate the tracing of a path and the description of interactions between elements of radiation and medium. Sample the probability distribution function for distance traveled and various probabilities to determine whether and what kind of radiation continues the process.
3. Repeat step 2 until either the radiation disappears (is absorbed) or becomes uninteresting.
4. During the iteration of step 2 count up interesting events to record physical results.

Steps 1–3 are, in effect, rules for carrying out a random walk of an object that moves from one point to another in a space of coordinates that describe the radiation. A minimal mathematical description of this requires four elements. First, we characterize the space on which the walk is defined. For present purposes, it can be R^n; some readers will find it convenient to visualize the random walk on the real line.

Second, we need a description (i.e. a probability distribution function) of the "source." This is a function

$$S(\boldsymbol{X}) \geq 0,$$
$$\int_\Omega S(\boldsymbol{X})\, \mathrm{d}\boldsymbol{X} = 1. \tag{5.49}$$

The normalization is convenient and, as will be seen, implies no loss of generality.

The third element is a stochastic rule for moving from one point (say $\boldsymbol{X}'$) to another (call it $\boldsymbol{X}$). This will be a distribution function $T(\boldsymbol{X}|\boldsymbol{X}')$ for sampling a new point $\boldsymbol{X}$ when the previous point of the walk was $\boldsymbol{X}'$. Note that a similar kind of transition distribution was introduced in Section 3.7 and again in Section 5.2 describing the $\mathrm{M(RT)}^2$ random walk. We shall require

$$T(\boldsymbol{X}|\boldsymbol{X}') \geq 0,$$
$$\int T(\boldsymbol{X}|\boldsymbol{X}')\, \mathrm{d}\boldsymbol{X} \leq 1. \tag{5.50}$$

That T is not normalized to 1 permits the possibility that the walk terminates (at $\boldsymbol{X}'$ with probability $1 - \int T(\boldsymbol{X}|\boldsymbol{X}')\, \mathrm{d}\boldsymbol{X}$).

The fourth element in our formulation is some variable of interest that we wish to know, at least conceptually. One general quantity will be the distribution of arrivals at $\boldsymbol{X}$, $\chi(\boldsymbol{X})$. That is, summing over all steps of the random walk and averaging over all possible walks, the expected number of times that a point is sampled within a region Ω is

$$\int_\Omega \chi(\boldsymbol{X})\, \mathrm{d}\boldsymbol{X}.$$

Recall that the walk starts with an $\boldsymbol{X}$ (call it $\boldsymbol{X}_0$) sampled from $S(\boldsymbol{X}_0)$. Then, if not absorbed[3], it moves to $\boldsymbol{X}_1$ sampled from $T(\boldsymbol{X}_1|\boldsymbol{X}_0)$. In general $T(\boldsymbol{X}_n|\boldsymbol{X}_{n-1})$ governs the nth move. The arrival at $\boldsymbol{X}$ can occur either because it was sampled from S or because it moved to $\boldsymbol{X}$ from an earlier point (call it $\boldsymbol{Y}$). The total average distribution at $\boldsymbol{X}$ is the sum of these two:

$$\chi(\boldsymbol{X}) = S(\boldsymbol{X}) + \int T(\boldsymbol{X}|\boldsymbol{Y})\chi(\boldsymbol{Y})\, \mathrm{d}\boldsymbol{Y}. \tag{5.51}$$

3) Absorption has the same meaning here as it did with Poisson processes; that is, the random walk ends.

The integral term on the right-hand side is the average distribution arrival at $\boldsymbol{X}$ from the next earlier arrival: $\chi(\boldsymbol{Y})\,\mathrm{d}\boldsymbol{Y}$ is the chance that there was an arrival in $\mathrm{d}\boldsymbol{Y}$; $T(\boldsymbol{X}|\boldsymbol{Y})$ is the probability that this was followed by a move to $\boldsymbol{X}$; one integrates over $\boldsymbol{Y}$ to average over all possible positions of the previous move.

Equation 5.51 is then an equation that describes the average behavior of the random walk. In a sense, since the outcome is a series of points $\boldsymbol{X}_0, \boldsymbol{X}_1, \boldsymbol{X}_2, \ldots$, the random walk can be regarded as a device for sampling the function χ that is the solution of Equation 5.51. This is analogous to the procedure used by M(RT)^2, but there is one vital difference. In the latter the distribution function was prescribed. Now, χ is in general unknown. In M(RT)^2 we did not use a specific S, and the correctness of the sampling is true asymptotically. Here S is part of the description, and the correctness of the sampling requires that every $\boldsymbol{X}_n$ generated in the walk be used. Like earlier sampling procedures, the set $\{\boldsymbol{X}_{nm}\}$ of points obtained from repetitions $m = 1, 2, \ldots, M$ of the whole random walk may be used to form estimators of integrals. That is, if

$$G = \int g(\boldsymbol{X})\chi(\boldsymbol{X})\,\mathrm{d}\boldsymbol{X}, \tag{5.52}$$

where χ is the solution of Equation 5.51, then the quantity

$$G_M = \frac{1}{M}\sum_{m=1}^{M}\sum_{n=1}^{N} g(\boldsymbol{X}_{nm}) \tag{5.53}$$

is an estimator for G in the (by now familiar) sense that

$$\langle G_M \rangle = G, \tag{5.54}$$

where the expectation implies averaging over all stochastic events that underlie the random walk.

5.3.2
The Boltzmann Equation

The fundamental equation that underlies the transport of radiation in matter is the Boltzmann equation and it expresses the equation of continuity:

production = losses + leakage.

Clearly, the ideas of Section 5.3.1 apply to the random walk that describes successive observations of radiation passing through matter. We use position $\boldsymbol{X}$, energy E, direction $\boldsymbol{\Omega}$, and time t to specify completely the state of the photon, neutron, etc. and call $\boldsymbol{P} = (\boldsymbol{X}, E, \boldsymbol{\Omega}, t)$ the point that characterizes that state. $\chi(\boldsymbol{P})$ will be the distribution with which radiation may be observed to emerge either from the source $S(\boldsymbol{P})$ or from a previous collision at $\boldsymbol{P}'$ followed by a flight from $\boldsymbol{X}'$ to $\boldsymbol{X}$ and a collision that changes E' to E and $\boldsymbol{\Omega}'$ to $\boldsymbol{\Omega}$. We shall call the transition distribution $K(\boldsymbol{P}' \to \boldsymbol{P})$ in this case. Then the ideas introduced in Section 5.3.1 transcribe to yield the integral equation

$$\chi(\boldsymbol{P})\,\mathrm{d}\boldsymbol{P} = S(\boldsymbol{P})\,\mathrm{d}\boldsymbol{P} + \int K(\boldsymbol{P}' \to \boldsymbol{P})\chi(\boldsymbol{P}')\,\mathrm{d}\boldsymbol{P}'\,\mathrm{d}\boldsymbol{P}. \tag{5.55}$$

The first term is simply the source contribution at $\boldsymbol{P}$. The second term is the average contribution from processes in which radiation emerging from a previous collision (or source) at $\boldsymbol{P}'$ arrives at $\boldsymbol{P}$ and emerges from collision there. The total radiation from the next collision is, of course, averaged over all possible $\boldsymbol{P}'$ that can contribute at $\boldsymbol{P}$. Equation 5.55 is the linear Boltzmann equation in integral form. The Monte Carlo simulation of radiation transport amounts to solving 5.55 by a random sampling method.

Any average quantity of interest that derives from radiation transport can be obtained by appropriate averages over $\chi(\boldsymbol{P})\,\mathrm{d}\boldsymbol{P}$. An expected value is defined as

$$G = \int g(\boldsymbol{P})\chi(\boldsymbol{P})\,\mathrm{d}\boldsymbol{P}, \tag{5.56}$$

where $g(\boldsymbol{P})$ is related to both the medium and the nature of the quantity to be determined. An estimator G_M may be formed as in Equation 5.53, which permits Monte Carlo computation of G to be made using the steps P_{nm} of the numerical random walks. A subject of considerable theoretical and practical interest is the formulation of functions $g(\boldsymbol{P})$ that permit results of engineering interest to be computed efficiently. We omit discussion of this here except for one trivial example: if one wishes to determine that fraction of radiation that escapes into a vacuum from a convex medium, one has only to count the cases where that occurs; that is, $g(\boldsymbol{P}) = 0$ when $\boldsymbol{X}$ is ''inside'' a medium and $g(\boldsymbol{P}) = 1$ when $\boldsymbol{X}$ is ''outside.'' The walk may be terminated on escape.

5.4 Variance Reduction

In many problems of interest the chance that the random walk reaches that region where an answer is obtained is small. The prototypical case is that mentioned at the end of Section 5.3.2: one wishes to calculate the escape of radiation from a ''thick'' medium in which many collisions must have an unlikely favorable outcome for the walk to contribute to the estimator. That is, for a fraction of steps very close to 1, $g(\boldsymbol{P})$ is 0. We seek methods to influence the random walk to make a favorable outcome rather likely.

5.4.1 Importance Sampling of Integral Equations

The problem has an analogy to importance sampling as used to reduce the variance in Monte Carlo quadrature (cf. Section 4.1). If

$$G = \int g(x)f(x)\,\mathrm{d}x$$

is to be calculated, sample $\tilde{f}(x)$ and rewrite

$$G = \int \frac{g(x)f(x)}{\tilde{f}(x)}\tilde{f}(x)\,\mathrm{d}x.$$

A favorable $\tilde{f}(x)$ will be one that is as nearly proportional to $|g(x)|f(x)$ as can technically be achieved. The Monte Carlo is improved when x is sampled so as to occur more often when the integrand is large, that is, when the contribution to the answer is large.

We shall employ a similar strategy here. First, we shall alter the distribution with which collisions are sampled in the hope of making them occur preferentially where contributions to the answer required are expected to be large. Second, we shall analyze what characterizes expected contributions. This is a more complicated question here since the random walk may have to make a number of steps in regions where $g(\boldsymbol{P}) = 0$ before arriving at a region where $g(\boldsymbol{P}) > 0$.

To achieve a modification of the collision distribution, we introduce an importance function $I(\boldsymbol{P}) \geq 0$ and multiply Equation 5.55 through by it. In the integral term, we multiply and divide by $I(\boldsymbol{P}')$ to obtain an integral equation for the product $I(\boldsymbol{P})\chi(\boldsymbol{P})$, which plays the role of an altered collision distribution.

Define S_0 by

$$S_0 = \int I(\boldsymbol{P}'')S(\boldsymbol{P}'')\,\mathrm{d}\boldsymbol{P}'';$$

then a new function $\tilde{\chi}(\boldsymbol{P})$ can be written in terms of S_0 and $I(\boldsymbol{P})$:

$$\begin{aligned}\tilde{\chi}(\boldsymbol{P}) &\equiv \frac{I(\boldsymbol{P})\chi(\boldsymbol{P})}{S_0} \\ &= \frac{S(\boldsymbol{P})I(\boldsymbol{P})}{S_0} + \int K(\boldsymbol{P}' \to \boldsymbol{P})\frac{I(\boldsymbol{P})}{I(\boldsymbol{P}')}\frac{I(\boldsymbol{P}')\chi(\boldsymbol{P}')\,\mathrm{d}\boldsymbol{P}'}{S_0}.\end{aligned} \tag{5.57}$$

This equation has the same formal structure as Equation 5.55, but the new source term is

$$\tilde{S}(\boldsymbol{P}) = \frac{S(\boldsymbol{P})I(\boldsymbol{P})}{S_0}, \tag{5.58}$$

which is normalized to 1. The modified kernel is

$$\tilde{K}(\boldsymbol{P}' \to \boldsymbol{P}) = \frac{K(\boldsymbol{P}' \to \boldsymbol{P})I(\boldsymbol{P})}{I(\boldsymbol{P}')}; \tag{5.59}$$

$I(\boldsymbol{P}')$ must not vanish when $K(\boldsymbol{P}' \to \boldsymbol{P})$ does not. If we use Equations 5.58 and 5.59, the integral equation in 5.57 becomes

$$\tilde{\chi}(\boldsymbol{P}) = \tilde{S}(\boldsymbol{P}) + \int \tilde{K}(\boldsymbol{P}' \to \boldsymbol{P})\tilde{\chi}(\boldsymbol{P}')\,\mathrm{d}\boldsymbol{P}', \tag{5.60}$$

and the definition of an expected value can be rewritten

$$G = \int g(\boldsymbol{P})\chi(\boldsymbol{P})\,\mathrm{d}\boldsymbol{P} = S_0 \int \frac{g(\boldsymbol{P})}{I(\boldsymbol{P})}\tilde{\chi}(\boldsymbol{P})\,\mathrm{d}\boldsymbol{P}, \tag{5.61}$$

with the further requirement that $I(\boldsymbol{P})$ cannot vanish when $g(\boldsymbol{P})$ does not. Any linear functional that could be evaluated using Equation 5.52 can be evaluated by means of Equation 5.61. The importance function modifies the path the radiation travels since the path from $\boldsymbol{P}'$ to $\boldsymbol{P}$ is now chosen from $\tilde{S}(\boldsymbol{P})$ and from $\tilde{K}(\boldsymbol{P}' \rightarrow \boldsymbol{P})$. For example, if $I(\boldsymbol{P}) > I(\boldsymbol{P}')$, the path will be biased toward $\boldsymbol{P}$.

References

1 Kirkpatrick, S., Gelatt, C.D. and Vecchi, M.P. (**1983**) Optimization by simulated annealing. *Science*, **220**, 671.

2 van Laarhoven, P.J. and Aarts, E.H. (**1987**) *Simulated Annealing: Theory and Applications (Mathematics and Its Applications)*, Springer-Verlag, New York.

3 Holland, J.H. (**1975**) *Adaptation in Natural and Artificial Systems*, University of Michigan Press, Ann Arbor, MI.

4 Kita, E., Tamaki, T. and Tanie, H. (**2004**) Structural design using genetic algorithm, in *Solid Mechanics and Its Applications*, Vol. 117 (eds T. Burczyński and A. Osyczka), Springer, Netherlands.

5 Taniguchi, E., Thompson, R.G., Yamada, T. *et al.* (eds) (**2001**) *City Logistics, Network Modelling and Intelligent Transport Systems*, Morgan Kaufmann, Burlington, MA.

6 Najim, K., Ikonen, E. and Daoud, A.-K. (**2004**) *Stochastic Processes Estimation, Optimisation and Analysis*, Morgan Kaufmann, Burlington, MA.

7 Spears, W. and Martin, W. (eds) (**2001**) *Foundations of Genetic Algorithms 2001*, Morgan Kaufmann, Burlington, MA.

8 Fogel, G. and Corne, D. (eds) (**2002**) *Evolutionary Computation in Bioinformatics*, Morgan Kaufman, Burlington, MA.

9 Nix, A.E. and Vose, M.D. (**1992**) Modeling genetic algorithms with Markov chains. *Annals of Mathematics and Artificial Intelligence*, **5**, 79.

10 Vose, M.D. (**1999**) *The Simple Genetic Algorithm: Foundations and Theory*, MIT Press, Cambridge, MA.

11 Wright, A.H. and Zhao, Y. (**1999**) Markov chain models of genetic algorithms, in *Proceedings of the Genetic and Evolutionary Computation Conference*, (eds W. Banzhaf, J. Daida, A.E. Eiben, *et al.*), Morgan Kaufmann, Burlington, MA.

12 Jain, R.J. and Jain, R.K. (**1991**) *The Art of Computer Systems Performance Analysis: Techniques for Experimental Design, Measurement, Simulation, and Modeling*, John Wiley & Sons, Inc., New York.

13 Spanier, J. and Gelbard, E.M. (**1969**) *Monte Carlo Principles and Neutron Transport*, Addison-Wesley, Reading, MA.

14 Howell, J.R. (**1968**) Application of Monte Carlo to heat transfer problems, in *Advances in Heat Transfer*, Vol. 5 (eds T.F. Irvine Jr. and J.P. Hartnett), Academic Press, New York.

15 Bertini, H.W. (**1976**) Spallation reactions: calculations, in *Spallation Nuclear Reactions and Their Applications*, (eds Chen B.S.P. and Merker M.), Reidel, Dordrecht, Boston.

16 Ayyub, B.M. and McCuen, R.H. (**2002**) *Probability, Statistics, and Reliability for Engineers and Scientists*, CRC Press, Boca Raton, FL.

17 Rubenstein, R.Y. (**1992**) *Monte Carlo Optimization, Simulation and*

Sensitivity of Queuing Networks, Krieger Publishing Company, Malabar, FL.

18 McLeish, D.L. (**2005**) *Monte Carlo Simulation and Finance*, John Wiley & Sons, Inc., New York.

19 Ross, S.M. (**2006**) *Simulation*, 4th edn, Elsevier Academic Press, Burlington, MA, San Diego, CA, London.

20 Law, A.M. and Kelton, W.D. (**1997**) *Simulation Modeling and Analysis*, 3rd edn, McGraw-Hill, New York.

Further Reading

Karlin, S. and Taylor, H.M. (**1975**) *A First Course in Stochastic Processes*, 2nd edn, Academic Press, New York.

6
Simulations of Stochastic Systems: Radiation Transport

In this chapter, we concentrate on simulations in just one area – the transport of radiation. This is a well-researched field [1–4], where much work has been done. The simulations use many of the techniques described previously in this book; it is apparent that these techniques are applicable in other fields as well.

6.1
Radiation Transport as a Stochastic Process

The transport of radiation is a natural stochastic process that is amenable to Monte Carlo modeling. To do so, it is not necessary even to write down the equations that are actually being solved as was done in Chapter 5. The particular simulation that is discussed in detail is a simplification of the naturally occurring process, and we first outline the assumptions and limitations of our model. We restrict ourselves to considering only neutral radiation such as light, X rays, neutrons, and neutrinos. The inclusion of charged particles such as electrons, protons, and alpha particles (nuclei of the ^{4}He atom) leads to a more complicated simulation since the radiation no longer travels straight-line paths between well-separated collisions. The details of the interaction of the radiation with the medium are greatly simplified, and we neglect the effect the radiation may have on the medium. For example, neutrons change most media through transmutation of the nuclei. For this reason, the composition of a nuclear reactor slowly changes with time, which will affect the paths of later neutrons. A feedback mechanism is established that makes the equations describing the radiation transport nonlinear. Monte Carlo methods are not generally effective for nonlinear problems mainly because expectations are linear in character. A nonlinear problem must usually be linearized in order to use Monte Carlo techniques. In most cases, the effect of transmutation is slow and the linearization is a good approximation.

We treat explicitly a simple geometry in discussing a simulation, but we sketch how more complicated geometries may be handled. Neutral radiation such as neutrons can be polarized since the neutron spin can have two different orientations, described as spin up or spin down. Neutrons scatter differently depending on their

Monte Carlo Methods. Second Edition. M.H. Kalos and P.A. Whitlock

ISBN: 978-3-527-40760-6

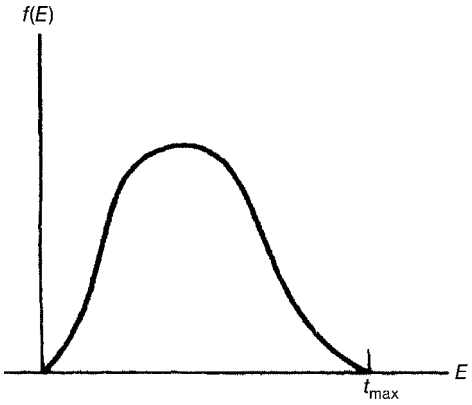


Figure 6.1 The energy distribution of the X-ray photons.

polarization, but this is not an important effect and is ignored here. Finally, we neglect crystal and similar effects on the transport of radiation. When the radiation has a wavelength equal to the crystal spacing, the radiation waves diffract and the pdf's for scattering change.

For the purposes of our discussion, we develop a simulation that models a familiar situation: the behavior of X-ray photons that are involved in a dental X-ray examination. These photons are initially produced by rapid deceleration of an electron beam. The energy distribution of the X rays varies from some lower limit to the highest energy of the electron beam, as shown in Figure 6.1. The energy of any individual photon cannot be predicted. The electron beam is focused on a target from which the X rays are emitted so the source is somewhat but not perfectly localized in space (Figure 6.2). The direction of the X rays is, to some extent, random. The electron beam is turned on and off as the X rays are needed so that they are not produced steadily in time.

The independent variables in the system detailed above are the energy, position, direction, and time of production of the photons. Each independent variable is random and may be described by a pdf. As X rays move through a vacuum, the spread in their direction makes their distribution decrease (asymptotically) proportional to R^{-2}. Once in matter, the photon may interact with an individual atom; whether an interaction takes place, and with which atom, is a random

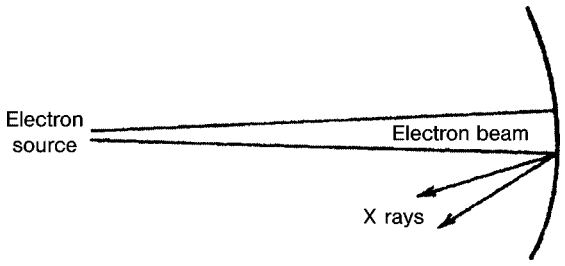


Figure 6.2 The collision of an electron beam on a target.

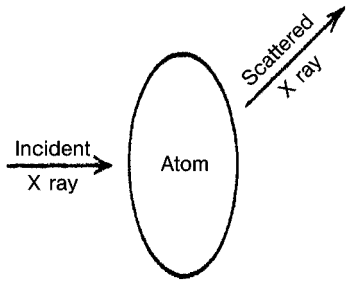


Figure 6.3 An X-ray scattering upon interaction with an atom.

process. The interaction usually involves the photons exchanging energy with an electron in the atom, which is effectively being scattered with reduced energy and changed direction (Figure 6.3). The photon may also give up all its energy to an electron, in which case it is considered to be absorbed and the history terminates. A relative probability based on knowledge of the relative rates is assigned to each event, scattering or absorption. An X-ray photon travels in straight lines until it interacts with an atom, at which point it may disappear or scatter at random. The scattered X ray is subject to the same processes as an original X ray of the same energy. In this and any other simulation, we must posit the pdf's governing each stochastic process that occurs. The distributions are deduced from theoretical and measured properties of X rays. In some cases, educated guesses are used to fill in gaps in the exact form of the distribution functions.

The life history of a photon is followed until the interest in it is lost or it is terminated. Termination occurs when a photon is absorbed by an atom. X rays that become too low in energy to have substantial later effects or that move far enough away to have no appreciable chance of influencing the required answer are also not considered. In summary, then, the process we wish to simulate is an X-ray photon born at a random position, direction, and time, which travels in straight-line segments whose lengths are random. The photon interacts with the atoms constituting the medium at random, and its life history is concluded at random.

An appropriate description of the radiation must be chosen for the simulation. X-ray radiation can be considered as an ensemble of X-ray photons and neutron radiation as an ensemble of individual neutrons. The simulation can be performed by following the life history of a single photon or neutron. To specify completely the state of an X-ray photon, the following variables are needed: three variables for the position, two or three for the direction, an energy variable, and a time variable. Thus, seven or eight independent variables are necessary.[1)] In practical calculations, three variables are generally used for direction rather than, say, a polar and azimuthal angle minimally needed. The values that the independent variables

1) When the geometry is simple, few variables may suffice. In slab geometry, one spatial coordinate and one direction variable are enough. In steady-state problems, time may be ignored.

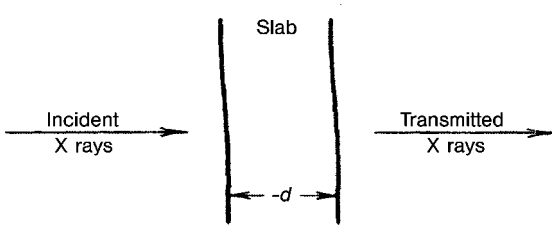


Figure 6.4 X rays incident upon a slab.

can assume determine an ensemble of states of the system. How do we describe the states? Is it necessary to sample all the states in the ensemble in our simulation?

To answer the last question, we need to state clearly our objectives in doing the simulation. For example, with regard to dental X rays, we can ask what dose of radiation is received at a particular position upon turning on the X rays at a prescribed voltage and for a known duration of time. Another possible objective in simulating X-ray transport would be to determine the fraction of radiation that passes through a slab of matter of known thickness d (Figure 6.4). Modeling of nuclear radiation might try to predict the number of neutrons produced within a reactor compared with the number introduced by an external source. A simulation of a laser beam passing through dust could be used to predict how much of the light is scattered and detected elsewhere. The information that is sought from the simulation will indicate which states of the system must be sampled.

As stated above, seven or eight variables may be used to specify uniquely the state of the radiation. The position coordinates may be taken as the Cartesian coordinates (x, y, z). The direction of the radiation can be specified by the direction cosines $(\Omega_x, \Omega_y, \Omega_z)$. If the radiation is a beam of neutrons, the direction cosines can be calculated from the particle velocities, for example,

$$\Omega_x = v_x/(v_x^2 + v_y^2 + v_z^2)^{1/2}.$$

An energy or equivalent variable must be given. In scattering visible light by an atom, the energy of the photon hardly changes. Also, in dental X rays, it is often the total dosage of radiation that is of interest, not the dosage as a function of time. This assumes, very reasonably, that the patient or technician does not move far as the photons traverse his or her body.

Once the system to be simulated has been clearly defined and the type of information wanted from the simulation is known, the structure of an appropriate code can be devised. For the simulation of dental X rays, a possible structure is as follows:

1. Pick a set of source variables (initial state of system).
2. Follow the X ray until it interacts with an atom.
3. Determine whether the X ray scatters.
   - if so, repeat from step 2;
   - if not, terminate the history.

Steps 2 and 3 are repeated until the X-ray photon is absorbed or is no longer capable of effecting the answer to any appreciable extent.

4. Repeat the whole process from step 1 as many times as necessary to achieve the accuracy needed for the solution.
5. Take arithmetic average of answers of all the histories.

6.2 Characterization of the Source

To realize step 1, sampling schemes must be developed for selecting the initial values of the independent variables from a source probability distribution function. In general, there exists a pdf for the production of radiation per unit volume, per unit direction, per unit energy, and per unit time:

$$S(x, y, z, \Omega_x, \Omega_y, \Omega_z, E, t).$$

We assume here that the source pdf can be factored into a product of pdf's, that is, position, direction, energy, and time are independent of one another:

$$S = S_x(x, y, z) S_\Omega(\mathbf{\Omega}) S_E(E) S_t(t). \tag{6.1}$$

This assumption simplifies our discussion; there are, however, important problems where factorization is not possible. In our simulation, we assume that the X rays are produced by what is termed a *point source*; that is, the X rays are created at the spatial point (x_0, y_0, z_0). We assume (incorrectly) that each photon has the same energy E_0. The variables (x, y, z) and E are then perfectly determined. The appropriate pdf's are

$$S_x = \delta(x - x_0)\,\delta(y - y_0)\,\delta(z - z_0) \tag{6.2a}$$

and

$$S_E = \delta(E - E_0). \tag{6.2b}$$

The X rays are produced by turning on the electron beam at t_1 and turning it off at t_2; this results in a pulse of X rays in the time interval $(t_2 - t_1)$ (Figure 6.5). We assume it to be constant during that period. The corresponding pdf is

$$S_t(t) = \begin{cases} \dfrac{1}{t_2 - t_1}, & t_1 < t < t_2 \\ 0, & \text{otherwise.} \end{cases}$$

We take the intensity of X rays to be uniform in all possible directions, so $S_\Omega(\mathbf{\Omega}) = \frac{1}{4\pi}$. In pseudocode, the sampling of the initial values of the system's independent variables for a point source is,

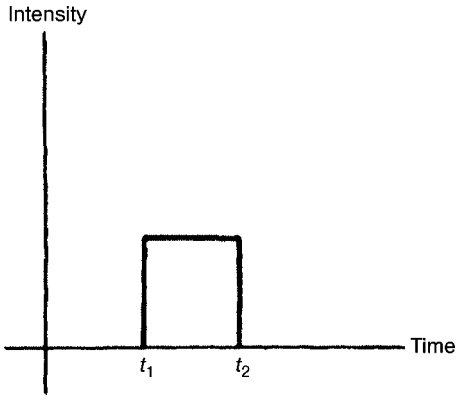


Figure 6.5 X-ray intensity as a function of time.

```
x = x0
y = y0
z = z0
energy = energy0
t0 = t2 + (t2 − t1)*rand(u)
phi = 2.*pi*rand(u)
omegaz = 1. − 2.*rand(u)
omegax = sqrt(1. − omegaz**2)*cos(phi)
omegay = omegax*tan(phi)
```

Again, it is assumed that each time the pseudorandom number generator, rand(), is called a new number is supplied. After some experience in simulation, one can code the selection of initial values without the necessity of writing down the source pdf's.

6.3 Tracing a Path

The next step is to follow the path of a photon until it has an interaction. The essential feature here is that X rays travel in straight lines until the interaction; so the change in position coordinates and time can be written down immediately as

$$x = x_0 + \Omega_x \times S,$$

$$y = y_0 + \Omega_y \times S,$$

$$z = z_0 + \Omega_z \times S,$$

$$t = t_0 + S/v,$$

where v is the radiation velocity and S is the distance to the next interaction with an atom. The probability per unit path length of having an interaction, Σ_T, is a

property of the material and does not change with the distance the photon has traveled, at least to the point where the medium changes:

$\Sigma_T(\boldsymbol{X}, E)$ = probability per unit length along the X-ray path for any interaction.

As a consequence, the distribution of the distances, S, is exponential in homogeneous materials. The probability $U(S|\boldsymbol{\Omega}, E, \boldsymbol{X}_0)$ that the first interaction is at $S' > S$ is conditional upon the initial values of $\boldsymbol{\Omega}$, E, and $\boldsymbol{X}_0$ through the properties of the materials that are encountered in the path. The function $U(S|\boldsymbol{\Omega}, E, \boldsymbol{X}_0)$ is the complement of a cumulative distribution. For the moment, we ignore the conditional dependencies of U and consider only its behavior with respect to S. The value of U at some S_1 can be written as

$$U(S_1) = U(S_2) + P\{S_2 \geq S > S_1\} \quad \text{for} \quad S_2 > S_1, \tag{6.3}$$

and $P\{\cdots\}$ is the probability that an interaction occurred between S_1 and S_2. Equation 6.3 may be rewritten as

$$U(S_1) - U(S_2) = U(S_1)P\{S_2 \geq S > S_1 | S > S_1\},$$

where $P\{\cdots\}$ is now the conditional probability that an interaction occurred if $S > S_1$. For small values of $S_2 - S_1$, the conditional probability that an event occurred is just the probability per unit length, $\Sigma_T(\boldsymbol{X}, E)$, multiplied by $(S_2 - S_1)$ plus higher-order terms:

$$U(S_1) - U(S_2) = U(S_1)\Sigma_T(S_1)(S_2 - S_1) + O(S_2 - S_1)^2. \tag{6.4}$$

Upon taking the derivative of Equation 6.4 with respect to S_2, we find

$$-U'(S) = U(S)\Sigma_T(S)$$

(the subscript on S has been dropped) or

$$\frac{-U'(S)}{U(S)} = -\frac{\mathrm{d}}{\mathrm{d}S}\log U(S) = \Sigma_T(S). \tag{6.5}$$

Equation 6.5 can be integrated to yield the distribution function for S,

$$-\log U(S) + \log U(0) = \int_0^S \Sigma_T(S')\,\mathrm{d}S'.$$

Since we know that exactly one interaction must take place for $S > 0$, $U(0) = 1$, and

$$U(S) = \exp\left[-\int_0^S \Sigma_T(S')\,\mathrm{d}S'\right]. \tag{6.6}$$

In a homogeneous medium, Σ_T is independent of S' so that

$$U(S) = \exp[-\Sigma_T S]; \tag{6.7}$$

therefore, the S's are indeed exponentially distributed.

Recall that $U(S)$ is the probability that an interaction takes place after a flight through a distance greater than S. We obtain a probability distribution function for the values of S by differentiating Equation 6.7:

$$\frac{-\mathrm{d}U(S)}{\mathrm{d}S} = \exp\left[-\int_0^S \Sigma_T(S')\,\mathrm{d}S'\right]\Sigma_T(S), \tag{6.8}$$

where the first factor on the right-hand side is the marginal probability that the path gets as far as S and the second term is the conditional probability that a collision occurs in $\mathrm{d}S$ at S. The distribution function is the probability of having a collision in a unit length along a ray at S.

For the purposes of the simulation, we need to decide how to sample the next event. As was discussed in Chapter 3, we can sample for a next event by equating a uniform random variable to a (cumulative) distribution function:

$$1 - U(S) = \xi' = 1 - \xi. \tag{6.9}$$

If the variable ξ is uniformly distributed, then $1 - \xi$ is also uniformly distributed and Equation 6.9 becomes

$$U(S) = \xi = \exp\left[-\int_0^S \Sigma_T(S')\,\mathrm{d}S'\right] \tag{6.10a}$$

or

$$-\log\xi = +\int_0^S \Sigma_T(S')\,\mathrm{d}S'. \tag{6.10b}$$

For the case of a homogeneous medium, $\Sigma_T(S)$ is constant, so

$$-\log\xi = \Sigma_T S \tag{6.11a}$$

and

$$S = -\log\xi/\Sigma_T. \tag{6.11b}$$

We must sample the distance S from an exponential distribution. (The same idea, that an event has a fixed chance to occur per unit time or distance or whatever no matter how long you wait, occurs in many circumstances. The idea has frequent application in queuing theory.) In most situations, the radiation travels through a medium that is a composite of several materials, each with its own value of Σ_T. Consider a ray and its direction in the medium as in Figure 6.6. To sample a next

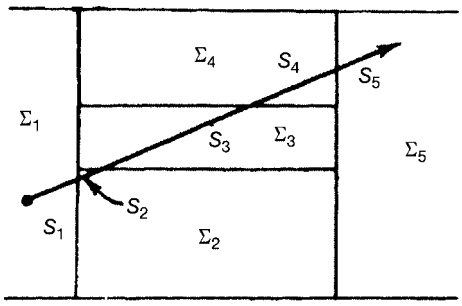


Figure 6.6 An X ray traveling through a composite medium.

event, we must locate each distance to a boundary between two media, for example, $S_1, S_2, \ldots$, with S being the total distance traversed. A uniform random number ξ is sampled and $-\log \xi$ is compared with $\Sigma_1 S_1$. If

$$-\log \xi < \Sigma_1 S_1, \quad \text{then} \quad -\log \xi = \Sigma_1 S, \quad \text{where } S < S_1;$$

else, test whether

$$\Sigma_1 S_1 < -\log \xi < \Sigma_1 S_1 + \Sigma_2 S_2; \quad -\log \xi = \Sigma_1 S_1 + \Sigma_2 (S - S_1),$$

where $S < S_1 + S_2$. That is, we want to find the ℓ such that

$$\sum_{j=1}^{\ell-1} \Sigma_j S_j \leq -\log \xi < \sum_{j=1}^{\ell} \Sigma_j S_j, \tag{6.12}$$

and then S is given by

$$S = \sum_{j=1}^{\ell-1} S_j - \frac{\left(\sum_{j=1}^{\ell-1} \Sigma_j S_j + \log \xi \right)}{\Sigma_\ell}, \tag{6.13}$$

where S_j is a partial distance in the jth medium encountered. The procedure is equivalent to finding that S where $-\log \xi$ intersects $\int_0^S \Sigma_T(S')\, dS'$ as shown in Figure 6.7. The procedure in Equation 6.12 is easily programmed recursively.

By using the type of analysis just described, it is very easy to sample for a next event in a complicated geometry. The major requirement is to be able to decide when a ray has intersected a surface. A quadric surface requires solving a quadratic equation; a linear surface requires solving a linear equation. The round-off error in such calculations can become serious, so that the intersections will be erroneously determined. The programming of a complicated geometry can be simplified by taking advantage of repetitive geometries, for example, latticelike structures. The ability to describe almost any geometry leads some naive users to include every nut and bolt in the simulation. This is clearly not necessary, and the user must be sufficiently objective and experienced to be able to decide what is important.

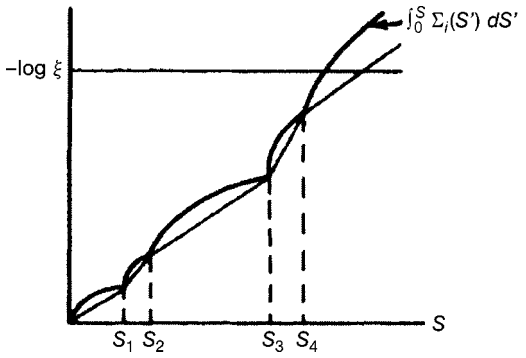


Figure 6.7 Finding the value of S where a next event will occur.

So far we have discussed the X-ray source, the appropriate means to sample initial coordinates at random, and the straight-line transport of neutral radiation. As mentioned earlier, charged radiation does not travel in straight-line paths but continually changes its direction with interactions. An electron is deflected when it passes an atom and in addition it steadily loses energy, which leads to winding paths. Though the description of the transport of charged radiation is technically more complicated than that of neutral radiation, the nature of the simulation parallels what we are discussing here [5].

6.4 Modeling Collision Events

Eventually, the neutral radiation does interact with the atoms of the substance it is passing through. The exact outcome of the collision depends on the nature of the radiation; for example, a light photon will usually scatter, whereas X-ray and γ-ray photons will interact with the atom in a more significant way. To model the collision, the first step is to enumerate the possible events, then assign a probability to each class of events, and finally decide which events are important enough to be included in the simulation.

Suppose only two events can occur upon collision. The radiation can be absorbed by the atom, which will then either re-emit some other radiation or convert the radiation energy to heat energy that is dissipated locally. For the moment, we suppose that our interest in the photon ceases upon absorption. The second event is the scattering of the radiation by the atom. The scattered radiation changes direction and loses energy, but for now we do not include the latter effect explicitly in our discussion. Now that we have enumerated the possible events, we can assign a probability for scattering and absorption for the radiation at its particular energy in the medium. If

$$\xi < \text{prob}\{\text{absorption}\}, \quad \text{absorption occurs;}$$

otherwise, a scattering event occurs. If scattering happens, then the path of the radiation is continued as before but the direction of flight may be changed, allowing collisions to occur at random until the radiation is absorbed or leaves the area of interest.

Both neutrons and X-ray photons tend to scatter preferentially in the forward direction in most materials; the azimuth is uniformly distributed (for unpolarized radiation). The coordinates appropriate for the scattered X rays are shown in Figure 6.8. The quantity $\mathbf{\Omega}$ is the unit vector in the old direction, θ is the scattering angle measured from $\mathbf{\Omega}$, and ϕ, the azimuthal angle, is chosen uniformly. In most simulations, $\cos\theta$ is the natural variable for the pdf. As an example, consider a material in which scattering is isotropic in the forward hemisphere; the appropriate distribution function is

$$f(\cos\theta)\, \mathrm{d}(\cos\theta) = \begin{cases} 2\cos\theta\, \mathrm{d}(\cos\theta), & 1 > \cos\theta > 0 \\ 0, & \cos\theta < 0. \end{cases}$$

Figure 6.8 The coordinates for the scattered X rays.

The new direction of the radiation is chosen by sampling $\cos\theta$ from the equations above and then sampling $\phi = 2\pi\xi$. The old direction cosines were $(\Omega'_x, \Omega'_y, \Omega'_z)$; the new direction cosines are given by

$$\begin{aligned}
\Omega_x &= \frac{\sin\theta}{\sqrt{1-\Omega_z'^2}}[\Omega'_y \sin\phi - \Omega'_z\Omega'_x \cos\phi] + \Omega'_x \cos\theta, \\
\Omega_y &= \frac{\sin\theta}{\sqrt{1-\Omega_z'^2}}[-\Omega'_x \sin\phi - \Omega'_z\Omega'_y \cos\phi] + \Omega'_y \cos\theta, \\
\Omega_z &= \sin\theta\sqrt{1-\Omega_z'^2}\cos\phi + \Omega'_z \cos\theta.
\end{aligned} \tag{6.14}$$

The set $(\Omega_x, \Omega_y, \Omega_z)$ is not unique – Equation 6.14 results from a particular choice of the origin of ϕ – but does satisfy

$$\boldsymbol{\Omega} \times \boldsymbol{\Omega}' = \cos\theta \tag{6.15a}$$

and

$$\Omega_x^2 + \Omega_y^2 + \Omega_z^2 = 1. \tag{6.15b}$$

Equations 6.14 are not stable numerically, and the normalization given in Equation 6.15b tends to drift from 1 after repeated usage of Equations 6.14. The $(\Omega_x, \Omega_y, \Omega_z)$ must be periodically renormalized. The von Neumann rejection technique (cf. Chapter 3) can be profitably used to choose $\sin\phi$ and $\cos\phi$, especially since they occur in association with a square root. If by chance $\Omega'_z = 1$, Equations 6.14 become indeterminant; this can be overcome by cyclic permutations of x, y, z in the equations. This change is also worth carrying out if Ω'_z is close enough to 1 to produce significant round-off error.

In addition to the two events discussed above, γ rays can also undergo a process termed *Compton scattering*, in which a γ ray photon interacts with an individual electron in the atom (Figure 6.9). The γ-ray is scattered, and the electron is ejected from the atom due to its increase in energy. Let E' be the energy of the γ-ray photon; then the *Compton wavelength* before scattering is

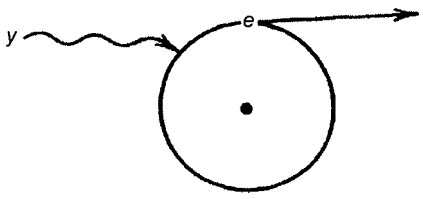


Figure 6.9 Compton scattering of γ rays.

$$\lambda' = \frac{m_e c^2}{E'}, \tag{6.16}$$

where m_e is the electron rest mass. Following scattering, the Compton wavelength will be designated by λ. The joint probability of being scattered into $d\lambda$ and a solid angle $d\boldsymbol{\Omega}$ is

$$d\sigma = \frac{3}{16\pi}\sigma_T \left[\left(\frac{\lambda'}{\lambda}\right)^2 \left\{ \frac{\lambda}{\lambda'} + \frac{\lambda'}{\lambda} + (\lambda' - \lambda)^2 - 2(\lambda - \lambda') \right\} \right] \times \delta(\cos\theta - 1 + \lambda - \lambda') \times d\boldsymbol{\Omega}\, d\lambda \tag{6.17}$$

where σ_T is termed the *Thomsen cross section*. The quantity $\delta(\cos\theta - 1 + \lambda - \lambda')$ is the Dirac delta function, which couples $\boldsymbol{\Omega}$ and λ as required by the conservation of energy and momentum. The expression in Equation 6.17 is the probability function for a γ-ray photon interacting with an electron and must be sampled in the simulation of γ rays. The Dirac delta function requires that

$$\lambda - \lambda' = 1 - \cos\theta \tag{6.18a}$$

or

$$\lambda = (1 - \cos\theta) + \lambda', \quad \cos\theta \geq 0, \tag{6.18b}$$

which is termed *Compton's law*. From Equation 6.18b we see that $\lambda > \lambda'$, so $E < E'$ (cf. Equation 6.16) and the γ-ray loses energy.

6.5 The Boltzmann Equation and Zero Variance Calculations

In Chapter 5, the characterization of the source, the tracing of the photon paths, and the modeling of collision events described above were shown to correspond to the integral form of the Boltzmann equation,

$$\chi(\boldsymbol{P})\, d\boldsymbol{P} = S(\boldsymbol{P})\, d\boldsymbol{P} + \int K(\boldsymbol{P}' \to \boldsymbol{P})\chi(\boldsymbol{P}')\, d\boldsymbol{P}'\, d\boldsymbol{P}, \tag{6.19}$$

where $\chi(\boldsymbol{P})$ is the distribution of arrivals at point $\boldsymbol{P}$. The term $S(\boldsymbol{P})\, d\boldsymbol{P}$ is the source contribution at $\boldsymbol{P} = (\boldsymbol{X}, E, \boldsymbol{\Omega}, t)$. The integral represents the average contribution from events in which radiation emerges from $\boldsymbol{P}'$, arrives at $\boldsymbol{P}$, and undergoes a collision there. It was further shown in Chapter 5 that the variance of some quantity of interest could be reduced by introducing an importance function into the integral equation. This idea is developed further to show that in principle importance sampling can lead to a zero variance calculation.

Suppose we are given an element of radiation somewhere. What is its chance of contributing to the quantity of interest? Let $J(\boldsymbol{P})$ equal the expected score (contribution to the quantity of interest) associated with radiation emerging from

a collision or the source at $\boldsymbol{P}$. The value of $J(\boldsymbol{P})$ is large where the radiation can ultimately score and is small elsewhere. $J(\boldsymbol{P})$ is called the importance since it assesses the likelihood of radiation at $\boldsymbol{P}$ to contribute to the score. An integral equation for $J(\boldsymbol{P})$ consistent with the above is

$$J(\boldsymbol{P}) = g(\boldsymbol{P}) + \int K(\boldsymbol{P} \to \boldsymbol{P}')J(\boldsymbol{P}')\,\mathrm{d}\boldsymbol{P}', \tag{6.20}$$

where $g(\boldsymbol{P})$ is the direct contribution to the score at $\boldsymbol{P}$. In addition, the radiation at $\boldsymbol{P}$ can have further collisions that may lead to contributions to the score or quantity of interest, G. The integral on the right-hand side is the average contribution from all possible positions $\boldsymbol{P}'$ that can be reached in a single collision after a collision at $\boldsymbol{P}$. Equation 6.20 is adjoint to Equation 6.19 for $\chi(\boldsymbol{P})$, and together the two equations form a dual. One manifestation of the duality is obtained by integrating both the equations;

$$\int \chi(\boldsymbol{P})J(\boldsymbol{P})\,\mathrm{d}\boldsymbol{P} = \int S(\boldsymbol{P})J(\boldsymbol{P})\,\mathrm{d}\boldsymbol{P} + \int\int J(\boldsymbol{P})K(\boldsymbol{P}' \to \boldsymbol{P})\chi(\boldsymbol{P}')\,\mathrm{d}\boldsymbol{P}'\,\mathrm{d}\boldsymbol{P},$$

$$\int J(\boldsymbol{P})\chi(\boldsymbol{P})\,\mathrm{d}\boldsymbol{P} = \int \chi(\boldsymbol{P})g(\boldsymbol{P})\,\mathrm{d}\boldsymbol{P} + \int\int \chi(\boldsymbol{P})K(\boldsymbol{P}- \to \boldsymbol{P}')J(\boldsymbol{P}')\,\mathrm{d}\boldsymbol{P}'\,\mathrm{d}\boldsymbol{P}.$$

The two double integrals are equal since $\boldsymbol{P}'$ and $\boldsymbol{P}$ are variables of integration and can be interchanged; hence,

$$\int \chi(\boldsymbol{P})g(\boldsymbol{P})\,\mathrm{d}\boldsymbol{P} = G = \int S(\boldsymbol{P})J(\boldsymbol{P})\,\mathrm{d}\boldsymbol{P}. \tag{6.21}$$

Either of the two integral equations in Equation 6.21 can be used to calculate G.

In the Monte Carlo sampling that uses $K(\boldsymbol{P}' \to \boldsymbol{P})$, the expected number of collisions following a collision at $\boldsymbol{P}'$ is

$$N(\boldsymbol{P}') = \int K(\boldsymbol{P}' \to \boldsymbol{P})\,\mathrm{d}\boldsymbol{P}. \tag{6.22}$$

$N(\boldsymbol{P}')$ is not easy to calculate in complicated situations; however, weighting by $J(\boldsymbol{P})$ we obtain a simple identity. The expected number of next collisions weighted by $J(\boldsymbol{P})$ is

$$N_J(\boldsymbol{P}') = \int \frac{J(\boldsymbol{P})K(\boldsymbol{P}' \to \boldsymbol{P})}{J(\boldsymbol{P}')}\mathrm{d}\boldsymbol{P}. \tag{6.23}$$

From Equation 6.20

$$\int J(\boldsymbol{P})K(\boldsymbol{P}' \to \boldsymbol{P})\,\mathrm{d}\boldsymbol{P} = J(\boldsymbol{P}') - g(\boldsymbol{P}'),$$

so

$$N_J(\boldsymbol{P}') = \frac{J(\boldsymbol{P}') - g(\boldsymbol{P}')}{J(\boldsymbol{P}')} = 1 - \frac{g(\boldsymbol{P}')}{J(\boldsymbol{P}')}. \tag{6.24}$$

One has $0 \leq g(\boldsymbol{P}') \geq J(\boldsymbol{P}')$ (cf. Equation 6.20) so that

$$0 \leq N_J(\boldsymbol{P}') \leq 1;$$

the expected number of next collisions is never greater than 1 when $\tilde{K}_J = K(\boldsymbol{P}' \rightarrow \boldsymbol{P})J(\boldsymbol{P})/J(\boldsymbol{P}')$ is used. $N_J(\boldsymbol{P}')$ can be viewed as the probability of continuing the random walk and $g(\boldsymbol{P}')/J(\boldsymbol{P}')$ as the probability of stopping. If

$$\frac{g(\boldsymbol{P}')}{J(\boldsymbol{P}')} = \frac{\text{current score contributions}}{\text{all future scores}}$$

is close to 1, then there is no need to go on. We use $N_J(\boldsymbol{P}')$ as the Monte Carlo probability for continuing the simulation from $\boldsymbol{P}'$, and the contribution to G will be calculated only when the walk stops (previously, we were estimating G at every collision). Scoring when the history ends means we score exactly once and it can easily be shown that a true zero variance estimator results. Note that zero variance calculations are possible for all linear Monte Carlo calculations, see Booth [6]. We write the estimator for G as

$$G = S_0 \sum \frac{g(\boldsymbol{P})}{J(\boldsymbol{P})}, \tag{6.25}$$

and evaluate Equation 6.25 with a $\boldsymbol{P}$ selected with probability $g(\boldsymbol{P})/J(\boldsymbol{P})$. Then the estimator is

$$S_0 \frac{g(\boldsymbol{P})}{J(\boldsymbol{P})} \times \left|\frac{g(\boldsymbol{P})}{J(\boldsymbol{P})}\right|^{-1} = S_0 = \int J(\boldsymbol{P}) S(\boldsymbol{P})\, \mathrm{d}\boldsymbol{P} = G. \tag{6.26}$$

The last equality is Equation 6.21. The estimate obtained from any history is G, independent of $\boldsymbol{P}$ and the whole preceding random walk, and is therefore a true zero variance estimator. It is necessary, unfortunately, that we already know the answer to the problem, $J(\boldsymbol{P})$, to evaluate Equation 6.26. We can still attempt to approach a zero variance calculation by using importance functions $I(\boldsymbol{P})$ (see Section 5.4.1) in the neighborhood of $J(\boldsymbol{P})$ and thereby reduce the variance of the Monte Carlo significantly. This idea is used extensively in radiation transport calculations.

6.5.1
Radiation Impinging on a Slab

As a simple illustration of these ideas, consider radiation impinging upon a thick slab of material, as shown in Figure 6.10. What fraction of the incidence radiation will emerge from the slab? The radiation is often observed empirically to decay nearly exponentially within the slab, so $\chi(z) \sim \mathrm{e}^{-\mu_0 z}$ (Figure 6.11). If we assume that the important radiation is that traveling normal to the slab, then a reasonable and simple choice of importance function is

$$I(z) \propto \mathrm{e}^{\mu_0 z}. \tag{6.27}$$

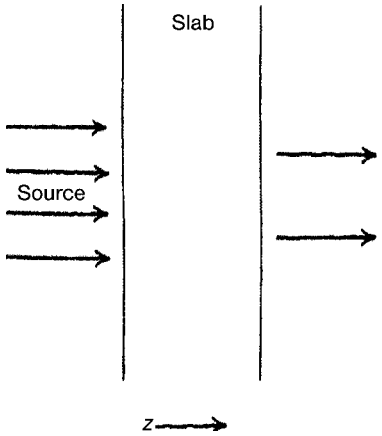


Figure 6.10 Radiation impinging on a slab of material.

This choice is correct only for radiation within the slab; its behavior beyond the slab is irrelevant since the random walk is terminated when the radiation exits. For radiation moving to the right in a direction making an angle with the normal whose cosine is ω,

$$K(z' \to z) = \left|\frac{\mu}{\omega}\right| \exp\left(\frac{-\mu(z-z')}{\omega}\right). \tag{6.28}$$

Then

$$\begin{aligned}\tilde{K}_I(z' \to z) &= K(z' \to z)\frac{I(z)}{I(z')} \\ &= |\mu/\omega| \exp\left[-(z-z')\left(\frac{\mu}{\omega} - \mu_0\right)\right],\end{aligned} \tag{6.29}$$

which is also an exponential and may be sampled in ways analogous to those used to sample z from K. The behavior of the effective attenuation coefficient in Equation 6.29,

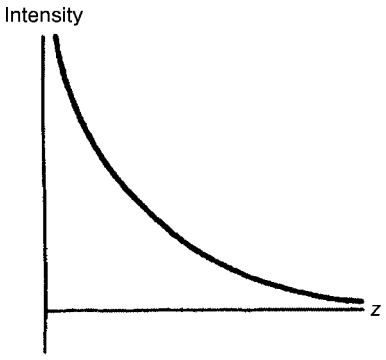


Figure 6.11 Radiation intensity within a slab.

$$\tilde{\mu} = \mu - \omega\mu_0, \tag{6.30}$$

as a function of ω is interesting. For $\omega = 1$ (radiation parallel to the slab normal), $\tilde{\mu} = \mu - \mu_0 < \mu$. Thus, for such paths, the effective attenuation is diminished and typical paths are "stretched" to encourage escape. For $\omega = -1$, $\tilde{\mu} = \mu + \mu_0 > \mu$. That is, for radiation moving back toward the source, paths are "shrunk" on the average to prevent their moving too far back and so diminishing their chances of contributing to the tally of escaping particles.

Note also that Equation 6.29 does not, unlike Equation 6.28, have the simple normalization such that $\int \tilde{K}_I(z)\, dz$ is necessarily less than 1. For radiation for which $\tilde{\mu} < \mu$, a branching or birth process – one particle turns into more on the average – is appropriate, and is an additional way in which a higher score is encouraged for radiation already likely to escape. Correct calculation of the required normalization permits one to pass through $\tilde{\mu} = 0$ without any singular behavior of the sampling procedure.

For practical purposes, the exponential in $I(z)$, Equation 6.27, may be approximated by a step function, as shown in Figure 6.12. $\tilde{K}_I(z)$ becomes the product of $K(z)$ and $I(z)$, as shown in Figure 6.13, if $I(z)$ balances $K(z)$ on the whole. The sawtooth kernel shown in the figure may be sampled in a variety of ways, but in any case it is necessary to take account of the fact that $\int \tilde{K}_I(z)\, dz$ may exceed 1. It is best to introduce branching, add a random walk, and so increase the chance of a score.

For a particle moving away from the slab exit, $\tilde{K}_I(z)$ is shown in Figure 6.14. The qualitative effect of $I(z)$ now reinforces that of $K(z)$ so that fewer particles are chosen for the continuation of the random walk and those that are chosen are closer, on the average, to z_0.

In general, the better that $I(\boldsymbol{P})$ approximates $J(\boldsymbol{P})$ and the sampling kernel approximates $I(\boldsymbol{P})K(\boldsymbol{P}' \to \boldsymbol{P})/I(\boldsymbol{P}')$, the more efficient the simulation is.

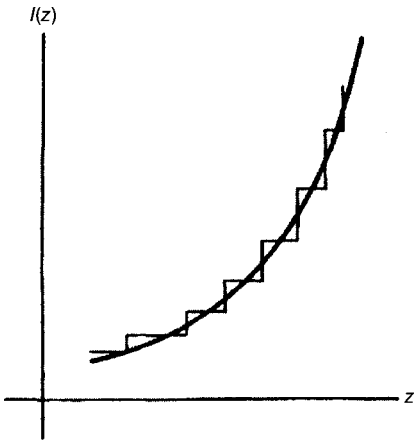


Figure 6.12 Approximating $I(z)$ by a step function.

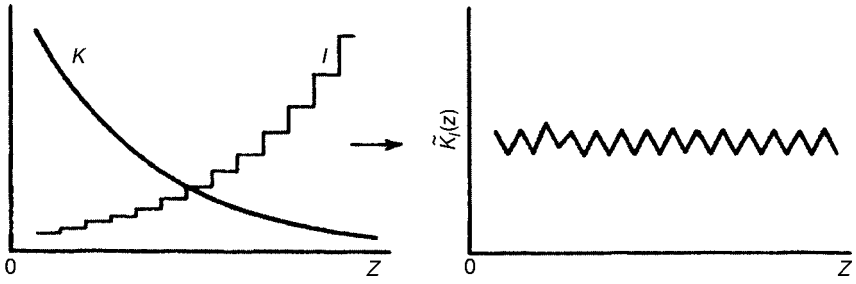


Figure 6.13 The product of $K(z)$ and $I(z)$.

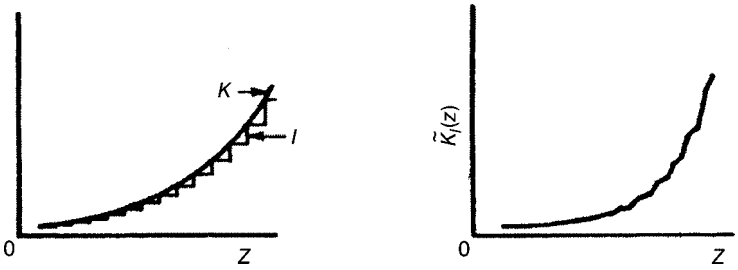


Figure 6.14 $\tilde{K}_I(z)$ for a particle moving backward from the slab exit.

References

1 Spanier, J. and Gelbard, E.M. (**1969**) *Monte Carlo Principles and Neutron Transport Problems*, Addison-Wesley, Reading, MA.

2 Carter, L.L. and Cashwell, E.D. (**1975**) *Particle Transport Simulation with the Monte Carlo Method, ERDA Critical Review Series*, TID-26607, Los Alamos National Laboratory, Los Alamos, NM, Available from the National Technical Information Service, U.S. Dept. of Commerce, Springfield, VA.

3 Lux, I. and Koblinger, L. (**1990**) *Monte Carlo Particle Transport Methods: Neutron and Photon Calculations*, CRC Press, Boca Raton, FL.

4 Dupree, S.A. and Fraley, S.K. (**2002**) *A Monte Carlo Primer: A Practical Approach to Radiation Transport*, Springer-Verlag, New York, LLC.

5 Berger, M.J. (**1963**) Diffusion of fast charged particles, in *Methods in Computational Physics*, Vol. 1 (eds B. Alder, S. Fernbach and M. Rotenburg), Academic Press, New York.

6 Booth, T.E. (**1989**) Zero-Variance Solutions for Linear Monte Carlo, *Nuclear Science and Engineering*, **102**, 332.

Further Reading

Goertzel, G. and Kalos, M.H. (**1958**) Monte Carlo methods in transport problems, *Progress in Nuclear Energy, Series I*, Vol. 2, Pergamon Press, New York, pp. 315–69.

Kling, A., Barao, F.J. and Nakagawa, M. (eds) (**2001**) *Advanced Monte Carlo for Radiation Physics, Particle Transport Simulation, and Applications*, Springer-Verlag, New York, LLC.

7
Statistical Physics

In this chapter and the next, we give introductions to Monte Carlo methods as they are used in specific applications in addition to radiation transport. This is, of course, important in itself, but many technical problems that arise in the applications are difficult to motivate out of context. Thus, in this chapter, we discuss applications in physics that require the evaluation of (usually very) many-dimensional integrals. The M(RT)^2 or Metropolis method, introduced in Section 3.7 is essential for practical treatment, so here we illustrate some technical points and discuss some of the scientific ideas that underlie the numerical simulations of physical systems.

7.1
Classical Systems

Suppose that $\boldsymbol{R}$ is a many dimensional vector whose associated probability distribution function is $f(\boldsymbol{R})$. The M(RT)^2 method constructs a random walk (cf. Section 5.2) such that the points $\boldsymbol{R}_i$ will eventually be drawn from $f(\boldsymbol{R})$. The random walk is initiated by choosing $\boldsymbol{R}_1$ from a pdf $\phi_1(\boldsymbol{R}_1)$. A possible next point is sampled using the transition distribution $T(\boldsymbol{R}_2'|\boldsymbol{R}_1)$ and the decision whether to accept $\boldsymbol{R}_2'$ is based on the quantity q, where

$$q = \frac{f(\boldsymbol{R}_2')T(\boldsymbol{R}_1|\boldsymbol{R}_2')}{f(\boldsymbol{R}_1)T(\boldsymbol{R}_2'|\boldsymbol{R}_1)}. \tag{7.1}$$

If $q > 1$, then $\boldsymbol{R}_2 = \boldsymbol{R}_2'$. If $q < 1$, $\boldsymbol{R}_2'$ is accepted with probability q; otherwise, $\boldsymbol{R}_2 = \boldsymbol{R}_1$. This process is repeated many times; each time a next $\boldsymbol{R}_i'$ is chosen from the transition distribution and accepted depending on the value of q. The eventual distribution of $\boldsymbol{R}$'s is guaranteed to be $f(\boldsymbol{R})/\int f(\boldsymbol{R})\,\mathrm{d}\boldsymbol{R}$.

Problems in statistical physics usually deal with the properties and characteristics of large ensembles of particles. For example, a classical situation [1] is N particles confined in a box. The configuration of the system may be represented by the multidimensional vector $\boldsymbol{R}$, which contains the $3N$ coordinates $\boldsymbol{r}_i = (x_i, y_i, z_i)$ of the centers of mass of the particles in the box. The total energy of the system is the sum of the kinetic energies of all the particles and the potential energy

Monte Carlo Methods. Second Edition. M.H. Kalos and P.A. Whitlock

ISBN: 978-3-527-40760-6

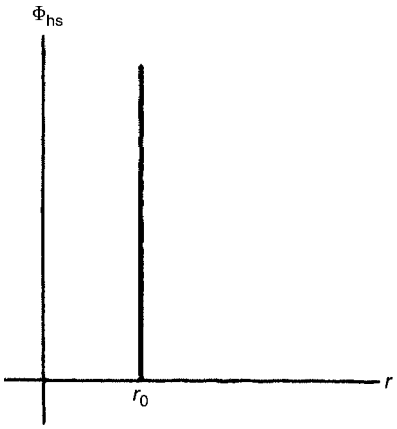


Figure 7.1 The hard sphere potential energy function.

$$E = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i=1}^{N-1} \sum_{j>i}^{N} \Phi(|\boldsymbol{r}_i - \boldsymbol{r}_j|). \tag{7.2}$$

Here p_i is the momentum and m_i is the mass of particle i. We have assumed that the total potential energy is the sum of the potential energies between a pair of particles.

Typical pair interaction forces used in calculations of this type are the hard sphere potential (shown in Figure 7.1):

$$\Phi_{hs}(r) = \begin{cases} \infty, & r < r_0 \\ 0, & r \geq r_0 \end{cases},$$

and the Lennard–Jones potential (shown in Figure 7.2)

$$\Phi_{LJ}(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right],$$

where r is the separation between two particles and ϵ and σ are parameters of the interaction. The Lennard–Jones force is a reasonably good representation of the pair potentials [2] in simple liquids such as helium, argon, and neon. The distribution of the particles in the box is a function of the particle positions and velocities:

$$f(v, \boldsymbol{R}) = \frac{\exp[-E(v, \boldsymbol{R})/k_B T]}{\int \exp[-E(v, \boldsymbol{R})/k_B T]\, d\boldsymbol{R}\, dv}, \tag{7.3}$$

where k_B is Boltzmann's constant, T is the temperature, and $E(v, \boldsymbol{R})$ is the energy of the system. At low temperatures, the particles will be close to some minimum energy configuration (solid) and at high temperatures ($T \to \infty$), $f(v, \boldsymbol{R}) =$ constant and the particles will be uniformly distributed as a gas. The distribution function in Equation 7.3 can be rewritten in terms of relative coordinates (interparticle separations, $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$) and the velocities can be integrated out to yield the Boltzmann distribution function

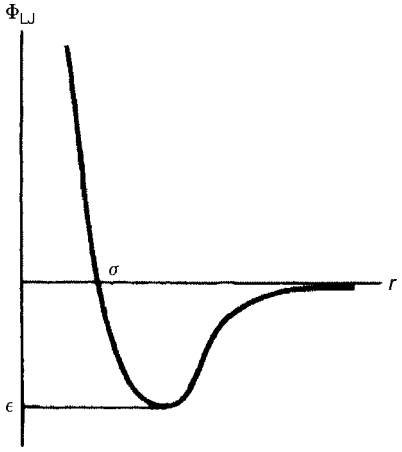


Figure 7.2 The Lennard–Jones potential energy function.

$$f(\boldsymbol{R}) = \frac{\exp\left[-\sum \Phi(r_{ij})/k_B T\right]}{\int \exp\left[-\sum \Phi(r_{ij})/k_B T\right] \mathrm{d}\boldsymbol{R}}. \tag{7.4}$$

We are now ready to determine the average energy of the particles, but we cannot do it analytically. A possible procedure is to sample $f(\boldsymbol{R})$ through the $\mathrm{M(RT)}^2$ method and determine the energy by Monte Carlo, that is, to estimate the average of $\sum_{i<j} \Phi(r_{ij})$.

7.1.1 The Hard Sphere Liquid

Suppose we have a hard sphere liquid in a three-dimensional box (Figure 7.3), where each hard sphere of diameter a moves in a cube of dimension Δ. As transition distribution in $\mathrm{M(RT)}^2$, we shall choose

$$T(\boldsymbol{R}'_n|\boldsymbol{R}_{n-1}) = \begin{cases} \frac{1}{\Delta^3} & \text{for } |x'_i - x_i|,\ |y'_i - y_i|,\ |z'_i - z_i| < \frac{\Delta}{2},\ \boldsymbol{r}'_j = \boldsymbol{r}_j,\ j \neq i, \\ 0 & \text{otherwise,} \end{cases}$$

where i is chosen at random from 1 to N. The constant transition distribution function drops out of the quotient for q (Equation 7.1). If a system can go from $\boldsymbol{R}_1$ to $\boldsymbol{R}'_2$, the reverse move is equally possible. Equation 7.1 becomes

$$q = \frac{\exp\left[-\sum \Phi(r'_{ij})/k_B T\right]}{\exp\left[-\sum \Phi(r_{ij})/k_B T\right]} = \exp\left[\frac{-\Delta U}{k_B T}\right],$$

where $\Delta U = \sum \Phi(r'_{ij}) - \sum \Phi(r_{ij})$. A move to a region of lower potential energy is automatically accepted; otherwise, the move is accepted with probability q.

In most cases, we are trying to model an infinite liquid, and the box size can have a dramatic effect on the final answer [3]. This may be partly overcome by using

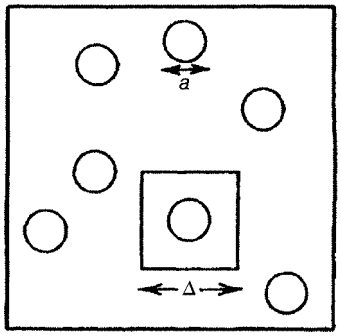


Figure 7.3 A two-dimensional slice through a hard sphere liquid.

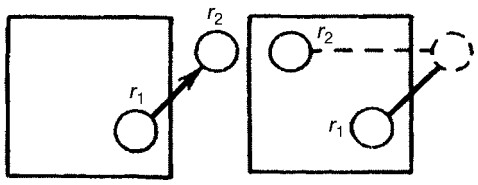


Figure 7.4 A particle moving beyond the edge of the box appears at its image position within the box.

periodic boundary conditions on the sides of the box. Periodic boundary conditions are illustrated in Figure 7.4. When a particle moves past the box on one side, it appears at the same position (less than the width of the box) on the ''opposite'' side. The coordinates of the particle are assigned to be those of the image position and the potential energy is computed using these coordinates obtained by translating through the dimensions of the box.

One property of the liquid that can be calculated through the Monte Carlo simulation is the pair correlation or radial distribution function. The pair correlation function $g(r)$ is the probability that two particles are a distance r apart:

$$g(r) = \left(1 - \frac{1}{N}\right)\left\langle \sum_{i<j} \delta(r - |\boldsymbol{r}_i - \boldsymbol{r}_j|) \right\rangle. \tag{7.5}$$

In the Monte Carlo simulation, it is determined by simply recording the frequency of occurrence of different particle separations in narrow bins. For hard spheres, $g(r)$ has the behavior that the particles tend to clump together such that many have an interparticle separation a little larger than the hard sphere diameter. This is shown in Figure 7.5. For nonhard sphere systems, the radial distribution function can be used to determine the potential energy of the system,

$$U = \frac{\rho}{2} \int g(r)\Phi(r)\, \mathrm{d}^3 r, \tag{7.6}$$

where ρ is the density of the system. Other properties of liquids that may be calculated during the random walk are the structure function $S(k)$ (the Fourier

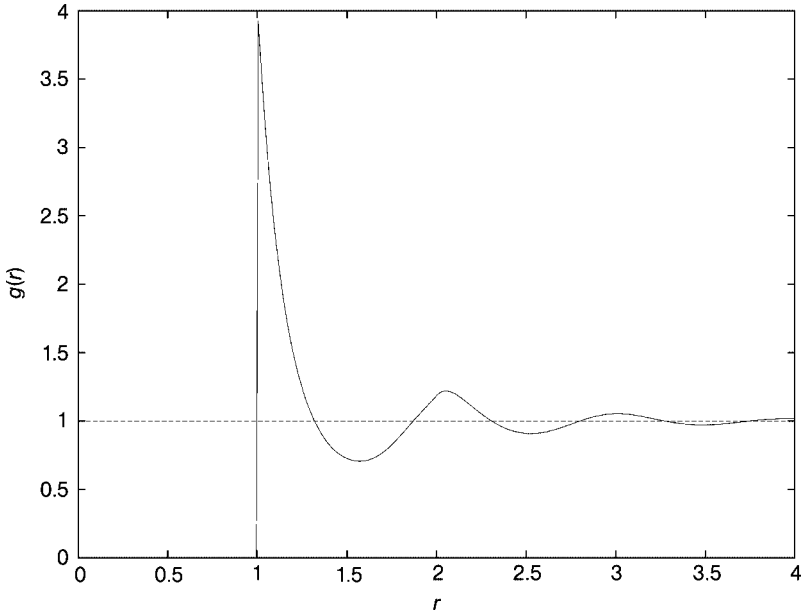


Figure 7.5 The radial distribution function for hard spheres.

transform of $g(r)$), the specific heat, and the density. However, it is not at all easy to directly determine A, the free energy of the system, by this kind of simulation:

$$Q = \exp\left[\frac{A}{k_B T}\right] = \frac{\int \exp\left[\frac{-\sum \Phi(r_{ij})}{k_B T}\right] d\boldsymbol{R}}{V^N}, \tag{7.7}$$

where V is the volume and Q is the canonical configuration integral. The free energy can be found using either a series of simulations at different temperatures [4] or a correlational Monte Carlo technique [5] that relates A for one system to the known A for a different one.

7.1.2 Molecular Dynamics

An alternative method used to study liquid systems is molecular dynamics [6]. In molecular dynamics, the motion of the particles is simulated by numerically solving Newton's equations for the system:

$$\boldsymbol{F} = m\frac{d\boldsymbol{v}_i}{dt} - \nabla_i \sum_{j<k} \Phi(r_{jk}), \tag{7.8}$$

where $\boldsymbol{v}_i$ is a particle velocity. The calculation is often started with the particles distributed on a lattice and initial velocities are randomly selected from the Boltzmann distribution

$$f(v) = \exp\left[\frac{-\frac{1}{2}mv^2}{k_B T}\right]. \tag{7.9}$$

The equations of motion are integrated in time to determine the paths the particles follow, and from this, time-dependent phenomena may be studied. For static correlation properties, however, Monte Carlo calculations are better since they generally converge faster to the probability distribution function $f(\boldsymbol{R})$. Also, the Monte Carlo calculations do not have to sample the entire phase space as is necessary in molecular dynamics calculations, since the integrations over momenta have already been done.

7.1.3 Kinetic Monte Carlo

Time-dependent phenomena in systems can also be studied by Monte Carlo techniques. That is, the dynamics of a multiparticle system may be simulated by creating a random walk that transits through the various successive states of the system. This type of random walk was introduced inSection 5.2.3. The straightforward translation of such a model is as a time-driven simulation, but as noted by Bortz *et al.* [7], an event-driven simulation is much more efficient in many applications.

Kinetic Monte Carlo [8] starts with a stochastic model of atomistic processes in dense materials, say, a solid. Simple examples are defined on a lattice in two or three dimensions and assume that some of the lattice points are occupied by one or more species of atoms. It is assumed that the probability for moving from one state i to another state of the system is an exponential distribution with a rate given by ω_i. Rates need to be specified for the addition, deletion, migration, or interaction of the atoms in the system and may be dependent upon the temperature of the system. The existence of all these possible events complicates a time-driven simulation but is easily taken into account when it is the next event that is sampled. In phenomenological terms, the event-driven simulation may be described as follows for the case where the rates of the different events are assumed to be independent of time:

1. Set the time to $t = 0$.
2. Create the list of all possible rates λ_i in the system.
3. Calculate the cumulative function $\Omega_i = \sum_{j=1}^{i} \lambda_j$ for $i = 1, \ldots, N$, where N is the total number of discrete events that can occur. This process is analogous to the description of sampling a discrete distribution function given in Section 3.3. Let $\Omega = \Omega_N$.
4. Choose the next event by sampling an i such that $\Omega_{i-1} < \xi_1 \cdot \Omega \leq \Omega_i$ where ξ_1 is a uniform random number.
5. Perform event i.

6. The rates may have changed owing to the occurrence of event i. Recalculate the affected rates and, if necessary, add new events, which will change the value of N.
7. Move forward in time as $t = t + \delta t$ where $\delta t = -\frac{\log \xi_2}{\Omega}$ and ξ_2 is also a uniform random number.
8. Evaluate the stopping criteria; if not satisfied, return to [2].

If the rates associated with the individual events are time dependent, the process described above needs to be modified to take the time dependence into account.

Fichthorn and Weinberg [9] have shown that the kinetic Monte Carlo method describes a Poisson process under the following conditions the different events are independent; detailed balance is present at equilibrium; and the time increment is calculated appropriately. If these criteria are met, then the probability of the system moving from state i to another state j is governed by the backward or forward Kolmogorov differential equations, Equations 5.36 and 5.37. A generalized version of these differential equations may be written as follows:

$$\frac{\mathrm{d}P_{ij}(t)}{\mathrm{d}t} = \sum_j K(X_i(t)|X_j(t-h))P_{ji}(t) - \sum_j K(X_j(t)|X_i(t-h)P_{ij}(t).$$

Kinetic Monte Carlo can, in principle, give the exact dynamical evolution of a system over large timescales. Of course, this ideal is rarely achieved and the algorithm listed above requires N operations for each transition from one state to another. Recently, a more sophisticated methodology, the first-passage technique [10], has proved to be much faster.

The major disadvantage with KMC is that all possible events and their associated rates have to be known in advance. The method itself can do nothing about predicting them.

7.1.4 The Ising Model

A very well-known model used in statistical physics is the Ising model [11] of interacting spins on a lattice. The model can be used to simulate the properties of a magnet. It is assumed that the spins can either be up or down with the value $+1$ associated with up and the value -1 associated with down:

$$\text{spin} = \sigma_i = \pm 1, \quad 1 \leq i \leq N,$$

where N is the number of particles. The total energy of the system is assumed to be

$$E = \sum_{i<j} J_{ij}\sigma_i\sigma_j + h\sum_{i=1}^{N}\sigma_i', \tag{7.10}$$

where the second term in Equation 7.10 derives from an external magnetic field of strength h. The quantity J_{ij} represents the interaction between nearest neighbors; the most commonly used assumption is

$$J_{ij} = \begin{cases} 0 & \text{if } i \text{ and } j \text{ are not nearest neighbors} \\ \text{constant} & \text{otherwise.} \end{cases}$$

The Ising model can be solved analytically [12] in two dimensions, but not in three. In either case, the Ising model exhibits a phase transition as the temperature is reduced from infinity. In three dimensions, this transition has interesting features in common with the critical point of a liquid. The Ising model is also used to model an alloy in which ''spins'' stand for one or another type of atom that may reside at a lattice site. Clusters of such atoms may develop, depending on the temperature. The $M(RT)^2$ method is commonly used, and various correlation functions can be extracted from the random walk.

Monte Carlo techniques have been used to exhaustively study systems obeying spherical potentials and are now being applied to more complicated systems. For example, surfaces can be studied by constructing a liquid and then removing the boundaries to form droplets [13]. A liquid like water can be simulated by Monte Carlo techniques that optimize the sampling [14] and by using more complicated potentials that are angle dependent [15]. Liquid crystals [16] are being studied by changing the particles in a box from spherical entities into rods, which take into account the peculiarities connected to the intrinsic properties of their mesophases.

References

1 Valleau, J.P. and Whittington, S.G. (**1976**) A guide to Monte Carlo for statistical mechanics: 1. Highways, in *Statistical Mechanics, Part A: Equilibrium Techniques*, *Modern Theoretical Chemistry Series*, Vol. 5 (ed B.J. Berne), Plenum, New York.

2 Barker, J.A. (**1976**) Interatomic potentials for inert gases from experimental data, in *Rare Gas Solids*, Chapter 4 (eds M.L. Klein and J.A. Verables), Academic Press, New York.

3 Metropolis, N., Rosenbluth, A.W., Rosenbluth, M.N. *et al.* (**1953**) Equations of state calculations by fast computing machines. *Journal of Chemical Physics*, **21**, 1087.

4 Valleau, J.P. and Card, D.N. (**1972**) Monte Carlo estimation of the free energy by multistage sampling. *Journal of Chemical Physics*, **57**, 5457.

5 Torrie, G. and Valleau, J.P. (**1974**) Monte Carlo free energy estimates using non-Boltzmann sampling. *Chemical Physics Letters*, **28**, 578.

6 Rappaport, D. (**2004**) *The Art of Molecular Dynamics*, 2nd edn, Cambridge University Press, Cambridge.

7 Bortz, A.B., Kalos, M.H. and Lebowitz, J.L. (**1975**) A new algorithm for Monte Carlo simulation of Ising spin systems. *Journal of Computational Physics*, **17**, 10.

8 Voter, A.F. (**2005**) Introduction to the kinetic Monte Carlo method, in *Radiation Effects in Solids* (eds K.E. Sickafus and E.A. Kotominin), Springer, NATO Publishing Unit, Dordrecht.

9 Fichthorn, K.A. and Weinberg, W.H. (**1991**) Theoretical foundations of dynamical Monte Carlo simulations. *Journal of Chemical Physics*, **95**, 1090.

10 Oppelstrup, T., Bulatov, V.V., Gilmer, G.H. *et al.* (**2006**) First passage Monte Carlo algorithm: diffusion without all the hops. *Physical Review Letters*, **97**, 230602.

11 Baxter, R.J. (**1982**) *Exactly Solved Models in Statistical Mechanics*, Academic Press, New York, pp. 14–23.

12 Baxter, R.J. (**1982**) *Exactly Solved Models in Statistical Mechanics*, Chapter 7, Academic Press, New York.
13 Neimark, A.V. and Vishnyakov, A. (**2005**) Monte Carlo simulation study of droplet nucleation. *Journal of Chemical Physics*, **122**, 174508–1.
14 Mezei, M. (**1987**) Grand-canonical ensemble Monte Carlo study of dense liquid Lennard-Jones, soft spheres and water. *Molecular Physics*, **61**, 565.
15 Errington, J.R. and Panagiotopoulos, A.Z. (**1998**) A fixed point charge model for water optimized to the vapor-liquid coexistence properties. *Journal of Physical Chemistry B*, **102**, 7470.
16 Pasini, P., Zumer, S. and Zannoni, C. (eds) (**2005**) *Computer Simulations of Liquid Crystals and Polymers, NATO Science Series II*, Springer-Verlag, New York, LLC.

Further Reading

Binder, K. and Heermann, D.W. (**2002**) *Monte Carlo Simulations in Statistical Physics*, 4th edn, Springer-Verlag, New York, LLC.
Landau, D.P. and Binder, K. (**2005**) *A Guide to Monte Carlo Simulations in Statistical Physics*, 2nd edn, Cambridge University Press, Cambridge.

8
Quantum Monte Carlo

The simulations described in Chapter 7 all assumed that the particles involved obey classical mechanics. It is also possible to study systems that are quantum mechanical in nature. The ground-state behavior of a quantum mechanical system is described by the Schrödinger equation

$$H\psi_0(\boldsymbol{R}) = E_0\psi_0(\boldsymbol{R}), \tag{8.1}$$

where H is the Hamiltonian for the system,

$$H = \sum_{i=1}^{N} -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j}\Phi(r_{ij}), \quad r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|,$$
$$\nabla_i^2 = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2}, \tag{8.2}$$

$\hbar$ is Planck's constant, $\psi_0(\boldsymbol{R})$ is the wave function, and E_0 is the ground-state energy. The quantity ∇_i^2 determines the kinetic energy of particle i, and $\Phi(r_{ij})$ represents the pair potential between particles i and j. At zero temperature, quantum particles are still in motion; this can be contrasted with classical mechanics, where particles are fixed at a minimum potential energy at zero temperature. The Schrödinger equation has been solved analytically only for the hydrogen atom; more complicated systems must be studied numerically.

In variational Monte Carlo (VMC) [1], knowledge of the physical relationships between the atoms can be built into a parametrized mathematical form for a trial wavefunction, $\psi_T(\boldsymbol{R})$, an approximation to the ground-state wavefunction, $\psi_0(\boldsymbol{R})$. The variational energy can be minimized with respect to the parameters through the Monte Carlo evaluation of the expectation value of the ground energy, E_0. Approaches where the Schrödinger or Bloch equations are modeled stochastically and are subject only to statistical uncertainties are referred to as Quantum Monte Carlo (QMC) methods. In the Green's function Monte Carlo (GFMC) method, introduced by Kalos [2, 3], the integral transform of the Schrödinger equation (Equation 8.1) is iterated by performing a random walk in the configuration space of N atoms to yield an asymptotically exact solution. Such a solution can also be obtained by sampling a short time Green's function followed by an extrapolation of the results to account

Monte Carlo Methods. Second Edition. M.H. Kalos and P.A. Whitlock

ISBN: 978-3-527-40760-6

for the time step errors introduced by the approximation. This technique is known as diffusion Monte Carlo (DMC) [4, 5]. Finally, finite temperature or imaginary time systems may be studied by considering the Bloch equation:

$$\left[-\nabla^2 + \Phi(\boldsymbol{R}) + \frac{\partial}{\partial\beta}\right]\psi(\boldsymbol{R},\beta) = 0. \tag{8.3}$$

Path integral Monte Carlo (PIMC) [6] simulations can be performed, and for small enough temperatures, the results can be compared to ground-state properties.

8.1 Variational Monte Carlo

For few-body and many-body systems, variational methods may be used to approximate the expectation values of system properties and the necessary integrals carried out by Monte Carlo [7]. If $\psi_T(\boldsymbol{R})$ is a trial wave function, the variational energy is defined as

$$E_{\text{var}} \equiv \frac{\int \psi_T(\boldsymbol{R}) H \psi_T(\boldsymbol{R})\, \mathrm{d}\boldsymbol{R}}{\int |\psi_T(\boldsymbol{R})|^2\, \mathrm{d}\boldsymbol{R}} \geq E_0. \tag{8.4}$$

That is, E_{var} is an upper bound to the ground-state energy. If $\psi_T(\boldsymbol{R}) = \psi_0(\boldsymbol{R})$, the actual wave function, then $E_{\text{var}} = E_0$. To use Monte Carlo techniques, the following probability distribution function is very convenient:

$$f(\boldsymbol{R}) = \frac{|\psi_T(\boldsymbol{R})|^2}{\int |\psi_T(\boldsymbol{R})|^2\, \mathrm{d}\boldsymbol{R}}, \tag{8.5}$$

and the variational energy (Equation 8.4) becomes

$$E_{\text{var}} = \int f(\boldsymbol{R}) E(\boldsymbol{R})\, \mathrm{d}\boldsymbol{R} = \langle E(\boldsymbol{R}) \rangle \geq E_0, \tag{8.6}$$

where $E(\boldsymbol{R})$ is the *local energy*, defined as

$$E(\boldsymbol{R}) = \frac{1}{\psi_T(\boldsymbol{R})} H \psi_T(\boldsymbol{R}). \tag{8.7}$$

To determine an estimate for E_{var}, values for $\boldsymbol{R}$ are sampled from $f(\boldsymbol{R})$, and the average of the resulting $E(\boldsymbol{R})$ is constructed. For systems with more than a few particles, the sampling can be done conveniently only with the M(RT)^2 method.

The Monte Carlo variational method has long been applied to liquid ^{4}He [1]. Liquid ^{4}He is a superfluid at low temperatures and solidifies only at high pressure; its properties must be obtained from a quantum mechanical calculation. As pointed out by Feenberg [8], a plausible general form for the exact ground-state wavefunction of a system of N interacting bosons is

$$\begin{aligned}\psi_T(\boldsymbol{R}) &= \prod_{i<j} f_2(r_{ij}) \prod_{i<j<k} f_3(i,j,k) \prod_{i<j<k<l} f_4(i,j,k,l) \cdots \\ &= \exp -\frac{1}{2}\left[\sum_{i<j} u(r_{ij}) + \sum_{i<j<k} u_3(i,j,k) + \sum_{i<j<k<l} u_4(i,j,k,l)\right] \cdots \end{aligned} \tag{8.8}$$

In the liquid phase, the simplest variational function, the so-called Bijl–Dingle–Jastrow or Jastrow trial function, considers only a single term of the above expression: $u_2(r_{ij})$. $u_2(r_{ij})$ is called the *pseudopotential* since it has a role similar to the potential in the Boltzmann distribution. The trial function becomes

$$\psi_T(\boldsymbol{R}) = \exp\left[-\frac{1}{2}\sum_{i<j} u_2(r_{ij})\right]. \tag{8.9}$$

The form of the pseudopotential is arbitrary as long as $u_2(\infty) = 0$, $u_2(0) = \infty$, and the first derivative is continuous. The actual representation for $u_2(r_{ij})$ is determined by minimizing E_{var}, with respect to the parameters in the functional form for u_2. By applying Green's theorem to Equation 8.6, E_{var} is written as

$$E_{\text{var}} = \frac{\rho}{2}\int \mathrm{d}^3 r\, g(r)\left(\Phi(r) + \frac{\hbar^2}{2m}\nabla^2 u_2(r)\right), \tag{8.10}$$

where ρ is the density of the system and $g(r)$ is the radial distribution function (Equation 7.5).

Liquid ^{4}He is a boson fluid, which means the wave function is symmetric upon interchange of two particle coordinates. Other interesting particles, for example electrons, are described by an antisymmetric wave function and are called *fermions*. The requirement of an antisymmetric wave function makes the description of fermions much more complicated. To treat fermions variationally, the following trial function has been used [9]:

$$\psi_T(\boldsymbol{R}) = \exp\left[-\sum_{i<j} u(r_{ij})\right] \times \det\left[\mathrm{e}^{\mathrm{i}\boldsymbol{k}_j\cdot\boldsymbol{r}_i}\right], \tag{8.11}$$

where det[$\cdots$] is the determinant of the ideal gas wave function:

$$\det\left[\mathrm{e}^{\mathrm{i}\boldsymbol{k}_j\cdot\boldsymbol{r}_i}\right] = \begin{vmatrix} \mathrm{e}^{\mathrm{i}\boldsymbol{k}_1\cdot\boldsymbol{r}_1} & \mathrm{e}^{\mathrm{i}\boldsymbol{k}_2\cdot\boldsymbol{r}_1} & \cdots \\ \mathrm{e}^{\mathrm{i}\boldsymbol{k}_1\cdot\boldsymbol{r}_2} & \mathrm{e}^{\mathrm{i}\boldsymbol{k}_2\cdot\boldsymbol{r}_2} & \cdots \\ \vdots & \vdots & \vdots \end{vmatrix}.$$

The $\boldsymbol{k}_i$ are momentum vectors in three-dimensional momentum space. When Equation 8.11 is used in the variational calculations, problems that are not present in a boson calculation occur. For example, $\psi_T(\boldsymbol{R})$ is occasionally equal to 0, which causes $E(\boldsymbol{R})$ to become infinite. Despite these and other difficulties, variational energies for a fermion system have been calculated by Monte Carlo techniques [9, 10]. Steady improvements in the form of variational wave functions have extended the systems investigated by VMC [11, 12].

8.2 Green's Function Monte Carlo

The power and importance of Green's function Monte Carlo [2, 3] is that it provides a means by which the Schrödinger [7] equation and the Bloch [13] equation may be

solved exactly for many-body boson [14] and also for fermion [15] systems. Since GFMC is a Monte Carlo method, the answers are subject to statistical sampling errors. For situations in which an exact answer to a quantum mechanical problem is desired, the GFMC method is a useful tool.

The essence of Green's function Monte Carlo can be described by four central ideas.

1. Monte Carlo methods can be used to solve integral equations, as was shown in the example of the treatment of radiation transport (Chapter 6).
2. The Schrödinger equation and the Bloch equation can be transformed into integral equations by using Green's function for an appropriate operator. This Green's function, though, is usually not known explicitly (i.e. in closed form).
3. Random walks, which occur in a Monte Carlo calculation, can be constructed to generate the required Green's functions. For example, the operator in the Bloch equation, $-\nabla^2 + V + \frac{\partial}{\partial\beta}$, describes a diffusion process. The simulation of diffusion processes on computers is a well-known application of Monte Carlo methods (cf. Chapter 5). It is not surprising, therefore, that the generation of Green's functions by random walks can be done by a computer-simulated stochastic process.
4. The statistical error inherent in a Monte Carlo calculation can be significantly reduced by introducing importance sampling. In principle, a calculation with importance sampling can have zero statistical error for a specific result (e.g. the energy of a quantum system).

8.2.1 Monte Carlo Solution of Homogeneous Integral Equations

We now develop the GFMC method, stressing the four ideas outlined above and in analogy with the developments in Sections 5.3, 5.4 and 6.5. Suppose the set of random variables $\{Y_1, Y_2, \ldots, Y_m, \ldots, Y_n\}$ is sampled from the distribution function $\chi(Y)$ in a volume V, and for each Y_m, another set $\{X_{m1}, X_{m2}, \ldots\}$ is drawn from $\lambda T(X|Y_m)$. The quantity λ is a known constant and T is an integrable, nonnegative function that serves as a distribution function for X conditional on Y. We call λT the *transition probability*; cf. Section 3.7 and the discussion of the M(RT)^2 algorithm. The average number of X_{mk} that are contained in V is

$$\langle N_{\{X_{mk}\in V\}}\rangle = \int_V \int \lambda T(X|Y_m)\chi(Y_m)\,\mathrm{d}Y_m\,\mathrm{d}X, \tag{8.12}$$

where

$\lambda T(X|Y_m)\,\mathrm{d}X =$ average number of X's in $\mathrm{d}X$,

$\chi(Y_m)\,\mathrm{d}Y_m =$ probability that $Y_m \in \mathrm{d}Y_m$.

Suppose that λ is an eigenvalue of the integral equation

$$\chi(X) = \lambda \int T(X|Y)\chi(Y)\,dY. \tag{8.13}$$

Equation 8.13 can be solved by the iterative sequence

$$\chi^{(n+1)}(X) = \lambda \int T(X|Y)\chi^{(n)}(Y)\,dY. \tag{8.14}$$

This is called a *Neumann series*, and the sequence converges to the distribution $\chi(X)$ that is the eigenfunction of Equation 8.13 having the smallest eigenvalue. Monte Carlo is used to iterate Equation 8.14 and is especially worthwhile when X and Y are many dimensional. The trial function or initial iterate $\chi^{(0)}(X)$ may be chosen to be a set of uniformly distributed random numbers. A better guess can be obtained from approximate solutions of the problem; variational calculations have proved especially useful (cf. Section 8.1).

So far, we have assumed that the eigenvalue is known but this is generally not the case. Let λ_T be an arbitrary (trial) value and λ denote the actual value. The trial value of λ_T is used instead of λ in the iterations of Equation 8.14. If $\lambda_T > \lambda$, the population of points X grows, since the size of the kernel is made larger; and if $\lambda_T < \lambda$, the population of X decays. This can be seen from Equation 8.12 since the expected number of points is proportional to λ. The choice of λ_T does not affect the convergence of the Neumann series to $\chi(Y)$ except insofar as the decay of the population may prevent the iteration from being continued. After the population converges, it is generally desirable to set λ_T so as to maintain approximately constant population size.

8.2.2
The Schrödinger Equation in Integral Form

We are interested in the ground-state energy and wave function $\psi_0(\boldsymbol{R})$ of the Schrödinger equation, Equation 8.1. The Green's function is defined by the equation[1)]

$$HG(\boldsymbol{R}, \boldsymbol{R}') = \delta(\boldsymbol{R} - \boldsymbol{R}') \tag{8.15}$$

with the same boundary conditions on $G(\boldsymbol{R}, \boldsymbol{R}')$ as on $\psi_0(\boldsymbol{R})$ for both $\boldsymbol{R}$ and $\boldsymbol{R}'$. The formal solution for the Green's function is

$$G(\boldsymbol{R}, \boldsymbol{R}') = \sum_{\alpha} E_a^{-1}\psi_\alpha(\boldsymbol{R})\psi_\alpha(\boldsymbol{R}'), \tag{8.16}$$

where the E_α are the eigenvalues and the $\psi_\alpha(\boldsymbol{R})$ are the eigenfunctions of the problem. We can rewrite the Schrödinger equation in the form of Equation 8.13,

1) Green's function as defined in Equation 8.15 may be either positive or negative. In the Monte Carlo calculation, we shall be sampling $G(\boldsymbol{R}, \boldsymbol{R}')$ and therefore require that it be nonnegative.

$$\psi_0(\boldsymbol{R}) = E_0 \int G(\boldsymbol{R}, \boldsymbol{R}')\psi_0(\boldsymbol{R}')\,\mathrm{d}\boldsymbol{R}', \tag{8.17}$$

and solve for $\psi_0(\boldsymbol{R})$ by iteration

$$\psi^{(n+1)}(R) = E_\mathrm{T} \int G(\boldsymbol{R}, \boldsymbol{R}')\psi^{(n)}(\boldsymbol{R}')\,\mathrm{d}\boldsymbol{R}', \tag{8.18}$$

where E_T is a trial energy. Suppose our initial distribution is $\psi^{(0)}(\boldsymbol{R})$. If we expand $\psi^{(0)}$ in the ψ_α,

$$\psi^{(0)}(\boldsymbol{R}) = \sum_\alpha C_\alpha \psi_\alpha(\boldsymbol{R}), \tag{8.19}$$

then by using Equations 8.16 and 8.17 we find that

$$\psi^{(n)}(\boldsymbol{R}) = \sum_\alpha \left(\frac{E_\mathrm{T}}{E_\alpha}\right)^n C_\alpha \psi_\alpha(\boldsymbol{R}). \tag{8.20}$$

For sufficiently large n, the term $\alpha = 0$ dominates the sum in Equation 8.20 and so

$$\psi^{(n)}(\boldsymbol{R}) \cong \left(\frac{E_\mathrm{T}}{E_0}\right)^n C_0 \psi_0(\boldsymbol{R}) \tag{8.21a}$$

and

$$\psi^{(n+1)}(\boldsymbol{R}) \cong \frac{E_\mathrm{T}}{E_0}\psi^{(n)}(\boldsymbol{R}). \tag{8.21b}$$

This result demonstrates that the iteration of Equation 8.18 will eventually give the ground-state wave function. The ground-state energy E_0 can be obtained from Equation 8.21b. It is worth reemphasizing that the Neumann series for solving an integral equation is applicable more generally. We are concerned with the use of Monte Carlo methods to perform the iterations.

The Green's function Monte Carlo method is easily demonstrated by using a simple example. Consider a one-dimensional particle on a line, enclosed by repulsive walls. The Schrödinger equation for this example is

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = E\psi(x), \quad \psi(x) = 0 \text{ for } |x| \geq 1. \tag{8.22}$$

The ground-state wave function and energy are

$$\psi_0(x) = \cos\left(\frac{\pi}{2}x\right), \quad E_0 = \left(\frac{\pi}{2}\right)^2, \tag{8.23}$$

and the appropriate Green's function is

$$G(x, x') = \begin{cases} \frac{1}{2}(1 - x')(1 + x), & x \leq x' \\ \frac{1}{2}(1 + x')(1 - x), & x \geq x'. \end{cases} \tag{8.24}$$

So, for a particular choice of x, the Green's function is piecewise linear, and the Green's function may be sampled separately for each linear portion. The integral equation we solve in this example is

$$\psi(x) = E_T \int_{-1}^{1} G(x, x')\psi(x')\, dx'. \tag{8.25}$$

$G(x, x')$ may be identified with $T(X|Y)$ of Section 8.2.1 and used as a distribution function. An iterative scheme can be described as follows. An initial population of points x' is chosen from $\psi^{(0)}(x')$; we assume it to be uniform. Then for each x', perform the following operations:

1. Construct the two triangles that form $G(x, x')$.
2. For each triangle, compute $E_T A$, where A is the area of the triangle.
3. For each triangle, generate a random integer N such that $\langle N \rangle = E_T A$ (i.e. $N =$ largest integer smaller than $E_T A$ plus a uniform random number).
4. Sample $\langle N \rangle$ points in each triangle to form the ''next generation.'' The points are sampled from a triangular-shaped probability distribution function normalized to 1.

In step 4, branching is used to form the next generation in the random walk. Alternatively, a weight, $E_T A$, could be associated with each new value of x and multiplied by the weight of x' in the previous generation. However, this latter method leads to the propagation of random walks with very uneven weights. In favorable areas, the weights become large, and in unfavorable regions, the weights approach zero. Branching avoids this problem by producing more random walks in the favorable regions without the necessity of tracking associated numerical weights.

8.2.3
Green's Functions from Random Walks

In our example, we have assumed that we know Green's function for the problem. In general, however, especially in many-dimensional problems, we do not. We can exploit the relationship with diffusion processes to construct the Green's function in problems where it is not known. Consider again the particle on a line; we show, using a suitable expansion (realizable as a random walk), that the required Green's function may be sampled.

Let us choose an isosceles triangle as a zero-order Green's function. That is, for any x' in $(-1, 1)$, $G_T(x, x')$ will be an isosceles triangle extending from x' to the nearest endpoint and an equal distance on the other side. This introduces an extra and erroneous cusp at $x = x_1$ (Figure 8.1). The correct Green's function has cusps only at $x = x'$ and at ± 1. We correct for the improper choice of $G_T(x, x')$ by adding a triangle at x_1 whose central cusp cancels the extraneous one. Since we assume that we do not know the correct Green's function, we approximate the correction by another isosceles triangle centered at $x = x_1$. If it has the right size, it cancels the first erroneous cusp while introducing a new extraneous cusp that we must cancel. In doing so, we define a (possibly) infinite sequence of iterations to sample $G(x, x')$ (Figure 8.2).

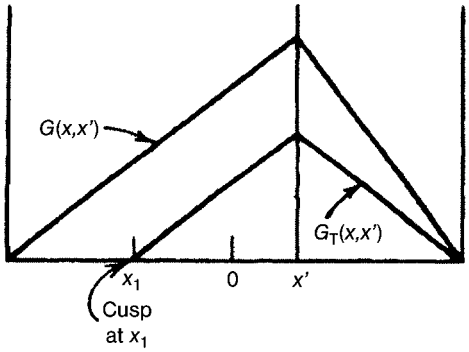


Figure 8.1 A $G_T(x, x')$ as an approximation to $G(x, x')$.

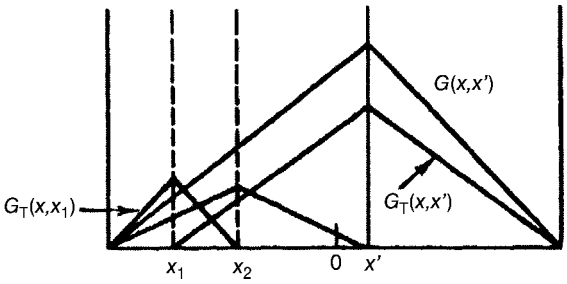


Figure 8.2 A sequence of functions $G_T(x, x_i)$ to sample $G(x, x')$.

A random subsequence may be sampled by means of a random walk. Depending on the values of the x_i, the random walk need not be infinite. A graphic illustration of a random walk with three iteration steps is shown in Figure 8.3. Since x_2 is equal to 0, the third isosceles triangle does not create any extraneous cusps and the random walk terminates.

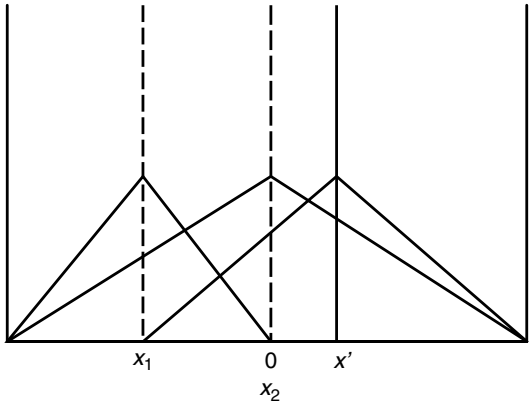


Figure 8.3 A random walk to sample $G(x, x')$ with three iterations.

The process described above in the one-dimensional example is mathematically formulated as follows. Let Green's function be defined as

$$-\nabla^2 G(\boldsymbol{R}, \boldsymbol{R}_0) = \delta(\boldsymbol{R} - \boldsymbol{R}_0). \tag{8.26a}$$

It can be shown that the solution is symmetric:

$$G(\boldsymbol{R}, \boldsymbol{R}_0) = G(\boldsymbol{R}_0, \boldsymbol{R}). \tag{8.26b}$$

For every $\boldsymbol{R}_1 \epsilon D$, construct a subdomain $D_u(\boldsymbol{R}_1) \subset D$ about $\boldsymbol{R}_1$ in such a way that the set of all D_u, $\{D_u\}$, covers the domain D. Within each D_u, we define a Green's function $G_u(\boldsymbol{R}, \boldsymbol{R}_1)$ by

$$-\nabla^2 G_u(\boldsymbol{R}, \boldsymbol{R}_1) = \delta(\boldsymbol{R} - \boldsymbol{R}_1) \tag{8.27a}$$

and

$$G_u(\boldsymbol{R}, \boldsymbol{R}_1) = 0 \quad \text{for } \boldsymbol{R}, \boldsymbol{R}_1 \notin D_u(\mathbf{R}_1). \tag{8.27b}$$

Now multiply Equation 8.26a by $G_u(\boldsymbol{R}_1, \boldsymbol{R}_0)$, multiply Equation 8.27a by $G(\boldsymbol{R}, \boldsymbol{R}_1)$, and subtract the two resulting equations. Integrate with respect to $\boldsymbol{R}_1 \in D_u(\boldsymbol{R}_0)$ and use Equation 8.27b to get

$$G(\boldsymbol{R}, \boldsymbol{R}_0) = G_u(\boldsymbol{R}, \boldsymbol{R}_0) + \int_{\partial D_u(\mathbf{R}_0)} [-\nabla_n G_u(\boldsymbol{R}_1, \boldsymbol{R}_0)] G(\boldsymbol{R}, \boldsymbol{R}_1)\, \mathrm{d}\boldsymbol{R}_1, \tag{8.28}$$

where $-\nabla_n$ is the outward directed normal derivative for $\boldsymbol{R}_1$ on the boundary of $D_u(\boldsymbol{R}_0)$. Equation 8.28 is a linear integral equation for $G(\boldsymbol{R}, \boldsymbol{R}_0)$ in terms of the known subdomain Green's function $G_u(\boldsymbol{R}, \boldsymbol{R}_0)$. We may integrate it by means of a random walk, which will deliver a set of values of $\boldsymbol{R}$ drawn from $G(\boldsymbol{R}, \boldsymbol{R}_0)$ (cf. Section 5.3). In our one-dimensional example, the equation becomes

$$G(x, x_0) = G_u(x, x_0) + \frac{\partial G_u(x, x_0)}{\partial x}\Big|_{x=x_1} G(x, x_1) \tag{8.29}$$

and $\frac{\partial G_u(x, x_0)}{\partial x}$ is the probability that a next triangle will be constructed at x. When this probability is small, the random walk is likely to be terminated. The points in the next generation, $\{x\}$, of the iterative solution to the original integral equation, Equation 8.25, are obtained by sampling $E_T \times G_u(x, x_1)$ for each point x_1 chosen in the random walk (Equation 8.29). Thus a random walk is generated for each x' in each generation that correctly samples $G(x, x')$ and evaluates Equation 8.25.

8.2.4
The Importance Sampling Transformation

The last technique that needs to be discussed in a general way is that of importance sampling. This is an example of the technique discussed earlier of transforming a problem into one that can be solved with lower, sometimes zero, Monte Carlo variance. In Chapter 4, the transformation appropriate for finite quadrature was introduced; in Chapter 5, the form required for variance reduction of integral

equations was developed; and in Chapter 6, the concept of a zero variance calculation in linear transport problems was discussed. In each case, it proved useful to multiply the distribution function to be sampled for a point $\boldsymbol{R}$ by an estimate of the answer to be expected as a result of using $\boldsymbol{R}_0$ (i.e. the ''importance'' at $\boldsymbol{R}_0$). For the present case of a homogeneous integral equation, we may ask, how do we estimate that importance? A point not likely to produce future points may be said to be *unimportant*. We propose then to use the expected contribution to the population after many generations from a point at $\boldsymbol{R}_0$ as the importance. This is easy to compute by iterating from the trial function

$$\psi^{(0)}(\boldsymbol{R}) = \delta(\boldsymbol{R} - \boldsymbol{R}_0) = \sum_\alpha \psi_\alpha(\boldsymbol{R})\psi_\alpha(\boldsymbol{R}_0), \tag{8.30}$$

where ψ_α are the eigenfunctions of the problem in Equation 8.1. Calculating the population after n iterates of the integral equation of Equation 8.18 gives

$$\psi^{(n)}(\boldsymbol{R}) = E_\mathrm{T}^n \sum_\alpha \frac{\psi_\alpha(\boldsymbol{R})\psi_\alpha(\boldsymbol{R}_0)}{E_\alpha^n} \; n \xrightarrow{} \infty \left(\frac{E_\mathrm{T}}{E_0}\right)^n \psi_0(\boldsymbol{R})\psi_0(\boldsymbol{R}_0). \tag{8.31}$$

The dependence of this on $\boldsymbol{R}$ reaffirms the convergence toward $\psi_0(\boldsymbol{R})$. The dependence on $\boldsymbol{R}_0$ shows the importance of a point at $\boldsymbol{R}_0$; that is, its relative contribution to the population after many generations is $\psi_0(\boldsymbol{R}_0)$.

We should, therefore, hope that introducing an integral equation for $\psi_0(\boldsymbol{R})\psi(\boldsymbol{R})$, rather than for $\psi(\boldsymbol{R})$, might lead to lower variance in the population, and hence in the energy estimate. That this anticipation is correct is seen as follows. Assuming $\psi_0(\boldsymbol{R})$ is a known function, one transforms Equation 8.18 into

$$\tilde{\psi}(\boldsymbol{R}) \equiv \psi_0(\boldsymbol{R})\psi(\boldsymbol{R}) = E_\mathrm{T} \int \left[\frac{\psi_0(\boldsymbol{R})G(\boldsymbol{R}, \boldsymbol{R}')}{\psi_0(\boldsymbol{R}')}\right] \tilde{\psi}(\boldsymbol{R}')\, \mathrm{d}\boldsymbol{R}'. \tag{8.32}$$

The nth iterate of this equation using $\delta(\boldsymbol{R} - \boldsymbol{R}_0)$ as initial function is again easily computed since the interior factors of $\psi_0(\boldsymbol{R})$ in the iterated kernel of the last equation cancel in pairs, leaving

$$\tilde{\psi}^n(\boldsymbol{R}) = E_\mathrm{T}^n \psi_0(\boldsymbol{R}) \sum_\alpha \frac{\psi_\alpha(\boldsymbol{R})}{E_\alpha^n} \to \left(\frac{E_\mathrm{T}}{E_0}\right)^n \psi_0^2(\boldsymbol{R}), \tag{8.33}$$

independent of $\boldsymbol{R}_0$. In fact, the expected size of the population after n steps is

$$N_n = \int \tilde{\psi}^{(n)}(\boldsymbol{R})\, \mathrm{d}\boldsymbol{R} = \left(\frac{E_\mathrm{T}}{E_0}\right)^n, \tag{8.34}$$

also independent of $\boldsymbol{R}_0$. If $E_\mathrm{T} = E_0$, the expected population size is strictly constant with n as well. Thus, it is possible to carry out the sampling (in the ideal case where $\psi_0(\boldsymbol{R})$ is known in advance) in such a way that the population size is precisely 1 at every stage. Thus, the energy as estimated from the population growth has zero variance.

For the one-dimensional problem, this means that sampling point x given x' should be carried out by using

$$\frac{\pi^2}{4}\left[\frac{\cos\left(\frac{\pi}{2}x\right)G(x,x')}{\cos\left(\frac{\pi}{2}x'\right)}\right] \tag{8.35}$$

as kernel. It is easy to verify that

$$\frac{\pi^2}{4}\int\left[\frac{\cos\left(\frac{\pi}{2}x\right)G(x,x')}{\cos\left(\frac{\pi}{2}x'\right)}\right]\mathrm{d}x = 1, \tag{8.36}$$

independent of x', which, in this case, is the explicit guarantee that the population has no statistical fluctuations.

The qualitative effect of the transformation is easy to understand. As $x' \to \pm 1$ for the particle in a box, the expected next population $E_T \int G(x,x')\,\mathrm{d}x \to 0$. By introducing $\cos\left(\frac{\pi x}{2}\right)$ as a factor in the distribution to be sampled, the number of points that turn up near $x = \pm 1$ is made small. At the same time, for those that do migrate near the wall, the contribution to the next generation is enhanced by the factor $\cos\left(\frac{\pi x'}{2}\right)$ that appears in the denominator of the modified kernel. The same balance will be obtained for the case of a general potential energy function when the appropriate $\psi_0(\boldsymbol{R})$ is used.

What has been established is that if ψ_0 is known and included as a *biasing factor* in the kernel and in the distribution to be sampled, it is possible to avoid most or all of the population size fluctuations. A practical procedure that suggests itself is to use some reasonable approximation to $\psi_0(\boldsymbol{R})$, which we call $\psi_T(\boldsymbol{R})$. Then introduce

$$\tilde{\psi}(\boldsymbol{R}) = \psi_T(\boldsymbol{R})\psi(\boldsymbol{R}) \tag{8.37}$$

and the transformed kernel is

$$\tilde{G}(\boldsymbol{R},\boldsymbol{R}') = \left[\frac{\psi_T(\boldsymbol{R})G(\boldsymbol{R},\boldsymbol{R}')}{\psi_T(\boldsymbol{R}')}\right]. \tag{8.38}$$

We expect that if $\psi_T(\boldsymbol{R})$ differs from $\psi_0(\boldsymbol{R})$ by a small amount, $\epsilon\psi_1(\boldsymbol{R})$, then the fluctuations in population and the variance of estimates of the energy will be $O(\epsilon^2)$. By now, much experience has shown that physically appropriate approximate functions, especially those whose parameters have been chosen by minimizing the energy or by matching known observables, reduce the Monte Carlo variance by very large ratios. In principle, the Monte Carlo calculation will give the same expected energy whatever be the importance function $\psi_T(\boldsymbol{R})$ that is used. In fact, a very poor and unphysical choice of $\psi_T(\boldsymbol{R})$ can make the Monte Carlo convergence slower, rather than faster, but this behavior, when it occurs, can usually be observed from the large fluctuations that accompany it. We note merely that appropriate avoidance of a hard wall or hard sphere potential is achieved by means of a trial function $\psi_T(\boldsymbol{R})$ that vanishes linearly in its neighborhood.

To apply the Green's function Monte Carlo method to fermion systems, the most usual approach is the "fixed-node" approximation [16, 17]. In this technique, an antisymmetric trial function, e.g. Equation 8.11, is used that has nodes, i.e.

subspaces of lower dimension on which they vanish. It can be shown that if the random walk is terminated when it reaches such a node, then the energy calculated for the system is an upper bound. This is widely used, and after several decades of development and optimization, very good results have been attained. Research into methods that are potentially as reliable as for bosonic systems is in process [18].

The calculations on light nuclei are noteworthy examples [19] in that the particle interactions here involve extremely complex nuclear forces. There are two-body forces derived from the study of nucleon–nucleon scattering, and these depend in complicated ways on the particles and their relative states. There are also three-body forces derived in a phenomenological way from the interactions of pions with nuclei. This means that a trial function for $A = 8$ comprises 17 920 complex functions. The quality of the agreement with experiment validates our understanding of the structure of nuclei at this level.

8.3 Diffusion Monte Carlo

An alternative approach to investigating quantum-mechanical systems involves the sampling of an approximate Green's function. The time-dependent Schrödinger equation in imaginary time $t \rightarrow \frac{\mathrm{i}t}{\hbar}$,

$$\frac{\partial\psi(\boldsymbol{R},t)}{\partial t} = -(-\nabla^2 + \Phi(\boldsymbol{R}) - E_\mathrm{T})\psi(\boldsymbol{R},t), \tag{8.39}$$

is equivalent to the classical diffusion equation, Equation 5.45, with sources represented by $\Phi(\boldsymbol{R})$. In Equation 8.39, the Hamiltonian H has been written as the sum of the kinetic energy T, $-\nabla^2$, plus the potential energy $\Phi(R)$ displaced by a trial energy E_T, which does not change the description of the state of the system.

In a short time approximation using the Trotter formula [20], the Green's function for Equation 8.39 can be written to $O(\delta t^2)$ as

$$G(\boldsymbol{R},\boldsymbol{R}',\delta t) \approx \langle \boldsymbol{R}|\mathrm{e}^{-\Phi(\mathbf{R})\delta t/2}\mathrm{e}^{-T\delta t}\mathrm{e}^{-\Phi(\mathbf{R}')\delta t/2}\mathrm{e}^{E_\mathrm{T}\delta t}|\boldsymbol{R}'\rangle. \tag{8.40}$$

It is possible to rewrite the above expression as the product of a rate term,

$$w(\boldsymbol{R},\boldsymbol{R}',\delta t) = \exp\left(-\left(\Phi(\boldsymbol{R}) + \Phi(\boldsymbol{R}')\right)\frac{\delta t}{2} + E_\mathrm{T}\delta t\right), \tag{8.41}$$

times a propagator, identified as the Green's function for ordinary diffusion,

$$G_\mathrm{d}(\boldsymbol{R},\boldsymbol{R}',\delta t) = \langle \boldsymbol{R}|\mathrm{e}^{-T\delta t}|\boldsymbol{R}'\rangle = (4\pi\delta t)^{-\frac{3N}{2}}\exp\left(-\frac{(\boldsymbol{R}-\boldsymbol{R}')^2}{4\delta t}\right). \tag{8.42}$$

In a simulation, for each $\boldsymbol{R}'$ in a given set of configurations, a new $\boldsymbol{R}$ is easily sampled from G_d using any method for sampling a Gaussian function (see Chapter 3). However, the probability for choosing the new value of $\boldsymbol{R}$ must be corrected by the rate term, Equation 8.41. This is accomplished by either assigning a weight to the random walk, which increases or decreases as each new value of $\boldsymbol{R}$ is sampled, or a birth/death propagation, branching, may be used to incorporate $w(\boldsymbol{R},\boldsymbol{R}',\delta t)$ into the random walk. In the latter case, a random integer,

$$\langle N \rangle = w(\boldsymbol{R}, \boldsymbol{R}', \delta t),$$

is chosen to decide how many copies (it may be zero) of the random walk continue in the next generation (see Section 8.2.2). By repeating these steps and performing a suitable extrapolation to $t \to 0$, the results will yield an estimate of the ground-state energy if $E_T \approx E_0$. This is shown by writing the formal solution of the time-dependent Schrödinger equation as

$$\psi(\boldsymbol{R}, t) = \sum_{\alpha} \psi_{\alpha}(\boldsymbol{R}) \mathrm{e}^{-\mathrm{i}(E_{\alpha} - E_T)\frac{t}{\hbar}}. \tag{8.43}$$

where the $\psi_{\alpha}(\boldsymbol{R})$ are an orthogonal basis set.

The method as described may be very inefficient owing to the branching process and because the random walk may explore unimportant regions of the configuration space. Here, again an importance sampling transformation as in Section 8.2.4 allows the simulations to converge faster and more efficiently. If Equation 8.39 is multiplied by a trial wavefunction ψ_T, it can be written in the coordinate representation as

$$\frac{\partial \tilde{\psi}(\boldsymbol{R}, t)}{\partial t} = -\left(-\nabla^2 + \nabla \cdot \boldsymbol{F}(\boldsymbol{R}) + \boldsymbol{F}(\boldsymbol{R}) \cdot \nabla - (E_T - E_L(\boldsymbol{R})\right) \tilde{\psi}(\boldsymbol{R}, t), \tag{8.44}$$

where $\tilde{\psi}(\boldsymbol{R}, t) = \psi_T(\boldsymbol{R})\psi(\boldsymbol{R}, t)$, $E_L(\boldsymbol{R})$ is the local energy, Equation 8.7, and $\boldsymbol{F}(\boldsymbol{R}) = 2\nabla \ln \psi_T(\boldsymbol{R})$. If we compare the above expression with Equation 8.39, it still includes a branching process, given by $\mathcal{V} = E_L(\boldsymbol{R}) - E_T$. The diffusion process has a superimposed drift velocity given by the two last terms of the expression, $-\nabla^2 + \nabla \cdot \boldsymbol{F}(\boldsymbol{R}) + \boldsymbol{F}(\boldsymbol{R}) \cdot \nabla$.
By taking the short time approximation, as before we can write:

$$\tilde{G}(\boldsymbol{R}, \boldsymbol{R}', \delta t) = \tilde{w}(\boldsymbol{R}, \boldsymbol{R}', \delta t)\tilde{G}_d(\boldsymbol{R}, \boldsymbol{R}', \delta t), \tag{8.45}$$

where

$$\tilde{w}(\boldsymbol{R}, \boldsymbol{R}', \delta t) = \exp\left(-(E_L(\boldsymbol{R}) + E_L(\boldsymbol{R}'))\frac{\delta t}{2} + E_T \delta t\right), \tag{8.46}$$

and

$$\tilde{G}_d(\boldsymbol{R}, \boldsymbol{R}', \delta t) = (4\pi\delta t)^{-\frac{3N}{2}} \exp\left(-\frac{(\boldsymbol{R} - \boldsymbol{R}' - \delta t \boldsymbol{F}(\boldsymbol{R}))^2}{4\delta t}\right). \tag{8.47}$$

Simulations that include importance sampling converge to $\psi_T(\boldsymbol{R})\psi(\boldsymbol{R})$. Instead of using $\Phi(\boldsymbol{R})$ to compute the rate term, E_L is now calculated, which approaches a constant as $\psi_T(\boldsymbol{R})$ converges to the true eigenfunction of the system. This is important since the simulations become much more stable. Moreover, the drift guides the random walk to the important regions of the configuration space.
The DMC algorithm may be summarized as follows:

1. Sample the first generation of points for the random walks from $\psi_T(\boldsymbol{R}')$.
2. For each value of $\boldsymbol{R}'$ in time interval δt, sample a value of $\boldsymbol{R}$ from Equation 8.47. That is, sample an $\boldsymbol{X}$ with mean 0 and variance $4\delta t$ and transform it to $\boldsymbol{R}$,

$$\boldsymbol{R} = \boldsymbol{X} + \boldsymbol{R}' + \delta t \boldsymbol{F}(\boldsymbol{R}').$$

3. For each value $\boldsymbol{R}$, generate an integer N such that

$$\langle N \rangle = \tilde{w}(\boldsymbol{R}, \boldsymbol{R}', \delta t),$$

   i.e. $N =$ largest integer smaller than $\tilde{w}$ plus a uniform random number.

4. Create $\langle N \rangle$ copies of $\boldsymbol{R}$ to form new random walks in the next generation.
5. Use the points $\{\boldsymbol{R}\}$ to calculate contributions to averages for expectation values.
6. Adjust E_T as needed to control the size of the population of random walks. Repeat steps 2–5 until the standard error of the estimators is acceptable.

The DMC method has been used extensively for both boson and fermion systems. To employ the method within the fixed-node approximation for fermion systems, development of very good trial wave functions is required. An example of a fermion system is the homogeneous electron gas [11]. The results for the electron gas are important for two reasons; they are the first highly reliable data for the equation of state of a many-electron system, and they form the basis of a very-widely used approximation method, ''density-functional theory.''

Another application that investigated fermion systems is the calculation of the energies of first-row dimers (i.e. Li_2 through F_2) [21]. To appreciate the nature of this achievement, one must first understand that the energy differences that are important for chemistry are of the order of 10^{-5} or less of the total energy of the system. Attaining this precision in a Monte Carlo calculation is evidence of sophisticated methodology. The second point is that the accuracy is very high, comparable or better than the ''traditional'' methods based on very large basis sets, an indication of the quality of the trial wave function optimization that is now possible.

8.4 Path Integral Monte Carlo

All static and, in principle, dynamic properties of a many-body quantum system, such as ^{4}He, at thermal equilibrium, may be obtained from the thermal density matrix, $\varrho(\boldsymbol{R}, \boldsymbol{R}', \beta)$, the propagator of the Bloch equation (8.3). β represents an inverse temperature or ''imaginary time,'' $\beta = \frac{1}{kT}$. The solution to the Bloch equation can be written in the coordinate representation as

$$\varrho(\boldsymbol{R}, \boldsymbol{R}', \beta) = \left\langle \boldsymbol{R} | e^{-\beta H} | \boldsymbol{R}' \right\rangle = \sum_{\alpha} \psi_{\alpha}^{\dagger}(\boldsymbol{R}) \psi_{\alpha}(\boldsymbol{R}) e^{-\beta E_{\alpha}}, \tag{8.48}$$

where ψ_α and E_α are the eigenfunctions and eigenvalues of the Hamiltonian, H. For distinguishable particles, the density matrix is nonnegative for all values of its arguments and can be interpreted as a probability distribution function. The expectation value of any property of interest, $\mathcal{O}$, is obtained as

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \varrho(\boldsymbol{R}, \boldsymbol{R}', \beta) \, \langle \boldsymbol{R} | \mathcal{O} | \boldsymbol{R}' \rangle \, \mathrm{d}\boldsymbol{R} \, \mathrm{d}\boldsymbol{R}', \tag{8.49}$$

where Z is the partition function and given by

$$Z = \int \varrho(\boldsymbol{R}, \boldsymbol{R}', \beta) \, \mathrm{d}\boldsymbol{R}.$$

If two density matrices are convoluted together, a density matrix at a lower temperature results:

$$\left\langle \boldsymbol{R} \left| \mathrm{e}^{-(\beta_1+\beta_2)H} \right| \boldsymbol{R}' \right\rangle = \int \left\langle \boldsymbol{R} \left| \mathrm{e}^{-\beta_1 H} \right| \boldsymbol{R}_1 \right\rangle \left\langle \boldsymbol{R}_1 \left| \mathrm{e}^{-\beta_2 H} \right| \boldsymbol{R}' \right\rangle \, \mathrm{d}\boldsymbol{R}_1. \tag{8.50}$$

The integral over $\boldsymbol{R}_1$ may be evaluated using a generalization of the Metropolis sampling algorithm [22]. Starting at a sufficiently high temperature, the density matrix may be written as an expansion in known one- and two-body density matrices. Multiple convolutions can be performed to reduce the temperature to near absolute zero. That is, let the total time β be divided into N time steps, $\frac{\beta}{N} = \delta\beta$. Then

$$\varrho(\boldsymbol{R}, \boldsymbol{R}', \beta) = \int \mathrm{d}\boldsymbol{R}_1 \, \mathrm{d}\boldsymbol{R}_2 \, \cdots \mathrm{d}\boldsymbol{R}_{N-1} \varrho(\boldsymbol{R}, \boldsymbol{R}_1, \delta\beta) \varrho(\boldsymbol{R}_1, \boldsymbol{R}_2, \delta\beta) \cdots \varrho(\boldsymbol{R}_{N-1}, \boldsymbol{R}', \delta\beta) \tag{8.51}$$

If N is finite, then the integrand in Equation 8.51 represents a discrete time path and is referred to as a *path integral* [23, 24]. Equation 8.51 is exact for any $N \geq 1$. In the limit $N \to \infty$, it becomes a continuous path beginning at $\boldsymbol{R}$ and ending at $\boldsymbol{R}'$.

To use Equation 8.51, a high temperature, small $\delta\beta$ form for the density matrix needs to be developed. An exact relationship for the operators $\mathcal{T} = -\nabla^2$ and Φ is given by

$$\mathrm{e}^{-\beta(\mathcal{T}+\Phi)+\frac{\beta^2}{2}[\mathcal{T},\Phi]} = \mathrm{e}^{-\beta\mathcal{T}} \mathrm{e}^{-\beta\Phi}. \tag{8.52}$$

As the imaginary time becomes small, the commutator term $\frac{\beta^2}{2}[\mathcal{T}, \Phi]$, which is of order β^2, can be neglected. This leads to the *primitive approximation*

$$\mathrm{e}^{-\delta\beta(\mathcal{T}+\Phi)} \approx \mathrm{e}^{-\delta\beta\mathcal{T}} \mathrm{e}^{-\delta\beta\Phi},$$

which allows the exact density matrix to be approximated by the product of matrices for $\mathcal{T}$ and Φ. That this is a valid approximation is justified by the Trotter formula [20]. That is, for small enough $\delta\beta$, $\mathrm{e}^{-\beta H}$ can be written as

$$\mathrm{e}^{-\beta(\mathcal{T}+\Phi(\mathbf{R}))} = \lim_{N\to\infty} \left(\mathrm{e}^{-\frac{\beta}{N}\mathcal{T}} \mathrm{e}^{-\frac{\beta}{N}\Phi(\mathbf{R})} \right)^N. \tag{8.53}$$

Separating the kinetic energy contribution from the potential energy contribution, Equation 8.51 may be rewritten using Equation 8.53 as

$$\begin{aligned} \varrho(\boldsymbol{R}, \boldsymbol{R}', \beta) = \int \cdots \int \mathrm{d}\boldsymbol{R}_1 \, \mathrm{d}\boldsymbol{R}_2 \, \cdots \mathrm{d}\boldsymbol{R}_{N-1} \langle \boldsymbol{R} | \mathrm{e}^{-\delta\beta\mathcal{T}} | \boldsymbol{R}_1 \rangle \, \cdots \, \langle \boldsymbol{R}_{N-1} | \mathrm{e}^{-\delta\beta\mathcal{T}} | \boldsymbol{R}' \rangle \\ \times \exp\left(-\delta\beta \sum_{i=1}^{N} \Phi(\boldsymbol{R}_i) \right), \end{aligned} \tag{8.54}$$

where $\boldsymbol{R}_N = \boldsymbol{R}'$. The free particle terms in Equation 8.54, which involve the kinetic energy contributions, can be viewed as a weight on all Brownian random walks that lead from $\boldsymbol{R}$ to $\boldsymbol{R}'$ in a time β. Designating these terms as $\varrho_0(\boldsymbol{R}, \boldsymbol{R}', \beta)$, Equation 8.54 can be rewritten in a Feynman–Kac relationship as

$$\varrho(\boldsymbol{R}, \boldsymbol{R}', \beta) = \varrho_0(\boldsymbol{R}, \boldsymbol{R}', \beta) \left\langle \exp\left(- \int_0^\beta \Phi(\boldsymbol{R}(\tau))\, \mathrm{d}\tau \right) \right\rangle. \tag{8.55}$$

The density matrix for a boson system such as ^{4}He is obtained from the distinguishable particle density matrix by using the permutation operator, $\wp$, to project out the symmetric component

$$\varrho(\boldsymbol{R}, \boldsymbol{R}', \beta) = \left\langle \boldsymbol{R} \left| \mathrm{e}^{-(\beta H)} \right| \boldsymbol{R}' \right\rangle_B = \frac{\sum_\wp \left\langle \wp \boldsymbol{R} \left| \mathrm{e}^{-(\beta H)} \right| \boldsymbol{R}' \right\rangle}{N!}. \tag{8.56}$$

The sum over permutations is also performed by a Monte Carlo technique.

Extensive calculations of the properties of ^{4}He at finite temperatures have been calculated and reviewed in [6]. To apply PIMC to fermion systems, one must restrict the paths to lie in regions where the fermion density matrix is positive [25].

Path Integral Ground State Calculations

Ground-state expectation values at finite temperatures can be efficiently calculated by using a path integral ground-state Monte Carlo method [26]. The integral equation in imaginary time equivalent to the Schrödinger equation is

$$\psi(\boldsymbol{R}, \beta) = \int G(\boldsymbol{R}, \boldsymbol{R}', \beta - \beta_0) \psi(\boldsymbol{R}', \beta_0)\, \mathrm{d}\boldsymbol{R}'. \tag{8.57}$$

In the above equation, $G(\boldsymbol{R}, \boldsymbol{R}', \beta)$ is the propagator of Equation 8.3. As was seen in the previous section, this propagator is viewed as a density matrix operator corresponding to an inverse temperature β and simulated by path integrals.

The difference in the present method compared to path integral Monte Carlo is that a truncated path on a trial wavefunction is considered instead of periodic boundary conditions in imaginary time, as the trace of $G(\boldsymbol{R}, \boldsymbol{R}', \beta)$ requires, Equation 8.49. Since the ground-state eigenfunction can be obtained by filtering a suitable trial function ψ_T,

$$\psi_0(\boldsymbol{R}) = \lim_{t \to \infty} \psi(\boldsymbol{R}, \beta) = \lim_{t \to \infty} \int G(\boldsymbol{R}, \boldsymbol{R}', \beta) \psi_\mathrm{T}(\boldsymbol{R}')\, \mathrm{d}\boldsymbol{R}', \tag{8.58}$$

the ground sate expectation value of any operator, $\mathcal{O}$, can be written as

$$\langle \mathcal{O} \rangle = \frac{\langle \psi_\mathrm{T}(\boldsymbol{R}) | G(\boldsymbol{R}, \boldsymbol{R}', \beta) \mathcal{O} G(\boldsymbol{R}, \boldsymbol{R}', \beta') | \psi_\mathrm{T}(\boldsymbol{R}') \rangle}{\langle \psi_\mathrm{T}(\boldsymbol{R}) | G(\boldsymbol{R}, \boldsymbol{R}', \beta) G(\boldsymbol{R}, \boldsymbol{R}', \beta') \psi_\mathrm{T}(\boldsymbol{R}') \rangle}. \tag{8.59}$$

If Equation 8.54 is substituted in Equation 8.59, we obtain

$$\langle \mathcal{O} \rangle = \frac{\displaystyle\int \prod_{i=0}^{N} \mathrm{d}\boldsymbol{R}_i \mathcal{O}(\boldsymbol{R}_i) \psi_\mathrm{T}(\boldsymbol{R}_0) \left(\prod_{i=0}^{N-1} \varrho(\boldsymbol{R}_i, \boldsymbol{R}_{i+1}, \delta\beta) \right) \psi_\mathrm{T}(\boldsymbol{R}_N)}{\displaystyle\int \prod_{i=0}^{N} \mathrm{d}R_i \psi_\mathrm{T}(\boldsymbol{R}_0) \left(\prod_{i=0}^{N-1} \varrho(\boldsymbol{R}_i, \boldsymbol{R}_{i+1}, \delta\beta) \right) \psi_\mathrm{T}(\boldsymbol{R}_N)}, \tag{8.60}$$

where $\boldsymbol{R}_0 = \boldsymbol{R}$, $\boldsymbol{R}_N = \boldsymbol{R}'$, and $\boldsymbol{R}_i$ is an internal time slice. For a converged calculation, if the operator is placed on the extreme edges of the path, one gets a mixed estimator. If $\boldsymbol{R}_i$ is in the middle, the exact expectation value of the ground state is obtained. The paths are sampled using the Metropolis algorithm. Samples that do not include coordinates of the trial wavefunction are performed as in path integral Monte Carlo.

8.5 Quantum Chromodynamics

Quantum chromodynamics (QCD) is the theory of the strong force that describes how quarks interact with gluons to form hadrons, the heavy particles that are the constituents of nuclear matter such as protons and neutrons [27]. It is a field theory, that is, it has a local symmetry described by a symmetry group, SU(3). Quantum electrodynamics is another example where the electrons and photons interact by way of fields based on the symmetry group U(1). Unlike electrodynamics where the intermediating particle is a photon, in QCD both the particles (quarks) and the quanta of the field (gluons) have many possible states. There are six types of quarks and eight gluons and the interactions of quarks and gluons and gluons with themselves are mediated by matrices that couple these different states. The coupling is strong so that the kind of perturbation theory that works well for electrodynamics does not converge in QCD. Fortunately, a discretized version of the theory, lattice gauge theory, which keeps the symmetry intact, was formulated by Wilson [28]. The discretization onto a lattice is a nonperturbative approximation that allows the containment of the divergences that occur in perturbative approaches and also can be systematically improved by increasing the lattice size and decreasing the spacings on the lattice. The method permits the direct numerical simulation of equilibrium properties of both the QCD phase transition and the high-temperature plasma phase.

In the lattice gauge theory approach, the four-dimensional space–time continuum is replaced by a four-dimensional hypercubic periodic lattice and the values of the quark fields are associated with the lattice sites. The gluon interactions are represented by the links. The computed result can be expressed as an average with respect to a weighting function. The quarks are fermions so that the weighting function is not positive, but reasonable approximation schemes can make it so. For example, in a recent formulation, called *domain wall fermions*, the fermionic fields are defined on a five-dimensional hypercubic lattice using a local action. The gauge fields are coupled to the extra fermion degrees of freedom in a diagonal way [29].

The numerical problem, for large enough lattices to approximate to a continuum, requires a Monte Carlo treatment. One such approach is labeled the ''Hybrid Monte Carlo'' method [30]. The partition function for a full-lattice QCD simulation is written as

$$Z = \int [\mathrm{d}U] \int [\mathrm{d}\overline{\Psi}\, \mathrm{d}\Psi] \int [\mathrm{d}\Phi^{\dagger}\, \mathrm{d}\Phi] \mathrm{e}^{-S}, \tag{8.61}$$

where $U(\boldsymbol{X})$ is the gauge field, $\Psi(\boldsymbol{X}, s)$ is the fermion field, and $\Phi(\boldsymbol{X}, s)$ is a bosonic Pauli–Villars field intended to cancel the contributions of heavy fermions. The variable $\boldsymbol{X}$ represents the coordinates in the four-dimensional lattice with an extent L along the spatial directions and an extent $\mathcal{T}$ along the time axis. The variable s, $s = 0, 1, \ldots, L_s - 1$, is the coordinate in the fifth dimension. The action S is defined as

$$S = S_{\mathrm{G}}(U) + S_{\mathrm{F}}(\overline{\Psi}, \Psi, U) + S_{\mathrm{PV}}(\Phi^{\dagger}, \Phi, U). \tag{8.62}$$

Here, $S_{\mathrm{G}}(U)$ is the purely gluonic standard plaquette action

$$S_{\mathrm{G}} = \beta \sum_{p} (1 - \tfrac{1}{3} ReTr U_{\mathrm{p}}),$$

with $\beta = 6/g_0^2$ and g_0 is the lattice gauge coupling. U_{p} is the product of the link matrices around an elementary square or plaquette on the lattice. The fermionic action for two flavors of fermions may be defined as

$$S_{\mathrm{F}} = - \sum_{\boldsymbol{X}, \boldsymbol{X}', s, s', f} \overline{\Psi}_f(\boldsymbol{X}, s) D_{\mathrm{F}}(\boldsymbol{X}, s; \boldsymbol{X}', s') \Psi_f(\boldsymbol{X}', s'); \quad f = 1, 2 \tag{8.63}$$

and D_{F} is, for example, the domain wall fermion Dirac operator [29]. S_{PV} is the Pauli–Villars action and has some flexibility in its definition.

To perform a simulation, the Hybrid Monte Carlo algorithm is constructed from Equation 8.62. The variables in the system evolve in a trajectory in time dynamically based on a stochastic Langevin method [31]. The particular dynamical trajectory is accepted or rejected by a M(RT)^2 algorithm based on the total energy change. All necessary matrix inversions are done using a conjugate gradient algorithm or related method.

Benchmark results have recently given the calculated masses of a range of hadrons [32] and large-scale calculations have extended results in the quenched QCD approximation [33]. Indeed, even after three decades of ingenious algorithmic development and more than 10^5 increase in computer speed, QCD continues to be a vibrant research area.

References

1 McMillan, W.L. (**1965**) Ground state of liquid ^{4}He. *Physical Review*, **138**, A442.

2 Kalos, M.H. (**1962**) Monte Carlo calculations of the ground state of three- and four-body nuclei. *Physical Review*, **128**, 1791.

3 Kalos, M.H., Levesque, D. and Verlet, L. (**1974**) Helium at zero temperature with hard-sphere and other forces. *Physical Review A*, **9**, 2178.

4 Ceperley, D.M. and Alder, B.J. (**1980**) Ground state of the electron gas by a stochastic method. *Physical Review Letters*, **45**, 566.

5 Ceperley, D.M. and Alder, B.J. (**1986**) Quantum Monte Carlo. *Science*, **231**, 555.

6 Ceperley, D.M. (**1995**) Path-Integrals in the theory of condensed helium. *Reviews of Modern Physics*, **67**, 279.

7 Ceperley, D.M. and Kalos, M.H. (**1979**) Quantum many-body problems, in *Monte Carlo Methods*

in Statistical Physics, Vol. 1 (ed K. Binder), Springer-Verlag, Berlin.
8 Feenberg, E. (**1974**) Ground state of an interacting bosons system. *Annals of Physics* (*N.Y.*), **84**, 128.
9 Ceperley, D.M., Chester, G.V. and Kalos, M.H. (**1977**) Monte Carlo simulation of a many fermion study. *Physical Review B*, **16**, 3081.
10 Moskowitz, J.W. and Kalos, M.H. (**1981**) A new look at correlations in atomic and molecular systems. I. Application of fermion Monte Carlo variational method. *International Journal of Quantum Chemistry*, **20**, 1107.
11 Kwon, Y., Ceperley, D.M. and Martin, R.M. (**1998**) Effects of backflow correlation in the three-dimensional electron gas: Quantum Monte Carlo study. *Physical Review B*, **58**, 6800.
12 Paris, M.W. (**2005**) Variational Monte Carlo study of pentaquark states. *Physical Review Letters*, **95**, 202002.
13 Whitlock, P.A. and Kalos, M.H. (**1979**) Monte Carlo calculation of the radial distribution function of quantum hard spheres at finite temperatures. *Journal of Computational Physics*, **30**, 361.
14 Schmidt, K.E., Niyaz, P., Vaught, A. *et al.* (**2005**) Green's function Monte Carlo method with exact imaginary-time propagation. *Physical Review E*, **71**, 016707.
15 Schmidt, K.E. and Kalos, M.H. (**1984**) Few- and many-body problems, in *Monte Carlo Methods in Statistical Physics*, Vol. 2 (ed K. Binder), Springer-Verlag, Berlin.
16 Anderson, J.B. (**1976**) Quantum chemistry by random walk. H^2P, H_3^+ D_{3h} $^1A_1'$, H_2 $^3\Sigma_u^+$, H_4 $^1\Sigma_g^+$, *Be* ^1S. *Journal of Chemical Physics*, **65**, 4121.
17 Arnow, D.M., Kalos, M.H., Lee, M.A. *et al.* (**1982**) Green's function Monte Carlo for few fermion problems. *Journal of Chemical Physics*, **77**, 5562.
18 Kalos, M.H. and Pederiva, F. (**2000**) Exact Monte Carlo method for continuum fermion systems. *Physical Review Letters*, **85**, 3547.
19 Pandharipande, V. (**2003**) Quantum Monte Carlo simulations of nuclei and nuclear reactions, in *The Monte Carlo Method in the Physical Sciences: Celebrating the* 50^{th} *Anniversary of the Metropolis Algorithm. AIP Conference Proceedings*, Vol. 690 (ed J.E. Gubernatis), American Institute of Physics, New York, 261.
20 Trotter, H.F. (**1959**) On the product of semi-group of operators. *Proceedings of the American Mathematical Society*, **10**, 545.
21 Umrigar, C.J., Toulouse, J., Filippi, C. *et al.* (**2007**) Alleviation of the fermion-sign problem by optimization of many-body wave functions. *Physical Review Letters*, **98**, 100201.
22 Pollock, E.L. and Ceperley, D.M. (**1984**) Simulation of quantum many-body systems by path-integral methods. *Physical Review B*, **30**, 2555.
23 Feynman, R.P. (**1953**) The lambda-transistion in liquid helium. *Physical Review*, **90**, 1116.
24 Kac, M. (**1959**) *Probability and Related Topics in Physical Science*, Interscience, New York.
25 Shumway, J. and Ceperley, D.M. (**2000**) Path Integral Monte Carlo simulations for fermion systems: pairing in the electron-hole plasma. *Journal de Physique IV*, **10**, 3.
26 Sarsa, A., Schmidt, K.E. and Magro, W.R. (**2000**) A path integral ground state method. *Journal of Chemical Physics*, **113**, 1366.
27 Quigg, C. (**1983**) *Gauge Theories of Strong, Weak, and Electromagnetic Interactions*, Addison Wesley Publishing Co.; Paperback, Westview Press, 1997.
28 Wilson, K.G. (**1974**) Confinement of quarks. *Physical Review D*, **10**, 2445.
29 Chen, P., Christ, N., Fleming, G. *et al.* (**2001**) The finite temperature QCD phase transition with domain wall fermions. *Physical Review D*, **64**, 014503.
30 Gottlieb, S., Liu, W., Toussaint, D. *et al.* (**1987**) Hybrid-molecular-dynamics algorithms for the numerical simulation of quantum chromodynamics. *Physical Review D*, **35**, 2531.

31 Batrouni, G.G., Katz, G.R., Kronfeld, A.S. *et al.* (**1985**) Langevin simulations of lattice field theories. *Physical Review D*, **32**, 2736.
32 Namekawa, Y., Aoki, S., Fukugita, M. *et al.* (**2004**) Light hadron spectroscopy in two-flavor QCD with small sea quark masses. *Physical Review D*, **70**, 074503.
33 Aoki, Y., Blum, T., Christ, N. *et al.* (**2005**) Lattice QCD with two dynamical flavors of domain wall fermions. *Physical Review D*, **72**, 114505.

Further Reading

Kalos, M.H. (ed) (**1984**) *Monte Carlo Methods in Quantum Problems*, D. Redidel, Dordrecht.
Nightingale, M.P. and Umrigar, C.J. (eds) (**1999**) *Quantum Monte Carlo Methods in Physics and Chemistry, NATO Advanced Science Institutes Series*, Springer-Verlag New York, LLC.
Suzuki, M. (ed) (**1993**) *Quantum Monte Carlo Methods in Condensed Matter Physics*, World Scientific, Singapore.

9
Pseudorandom Numbers

In much of the discussion on why and how to perform calculations using Monte Carlo methods, reference is made to a special type of random variable, the uniform random number ξ. This variable is expected to be distributed between $(0, 1)$ with the property that

$$P\{\xi < x\} = x, x \in (0, 1). \tag{9.1}$$

Once we have a source of uniform random numbers, we can sample any other pdf and carry out Monte Carlo integrations and simulations. Thus it would appear that we must find such a source.

Since our interest lies in the use of Monte Carlo methods on computers, our source of uniform random variables must be capable of delivering them at the rate needed by a high-speed calculation. There are Monte Carlo calculations and some simulations in which the computation rate is dominated by the rate at which random numbers can be produced. Rejection techniques are often random-number intensive. Clearly, one should avoid a procedure in which random numbers take (say) a millisecond to produce on a machine that can do billions of floating-point operations per second. Most natural sources of random events do not supply the events at such a rate (neglecting the difficulty of interfacing the source and the computer), and one would need an enormous table of previously compiled random numbers to complete a large calculation. Furthermore, we really want to be able to repeat our calculation at will, for debugging purposes and for various correlated sampling schemes. Thus, for most calculational purposes, pseudorandom numbers (prn's) are employed. Pseudorandom numbers are sequences of numbers on $(0, 1)$ that are easily generated on the computer and that will satisfy some statistical tests for randomness. Since the prn's are computed from a deterministic algorithm, they are not truly random and therefore cannot pass every possible statistical test[1)] The important criterion is that the pseudorandom number generator (prng) used in a calculation satisfies those statistical tests that are most closely related to the problem being studied [2–5]. The use of test problems whose exact answers are known is also desirable.

1) It may seem that we are glossing over the fact that prn's are not truly random. However, see [1].

Monte Carlo Methods. Second Edition. M.H. Kalos and P.A. Whitlock

ISBN: 978-3-527-40760-6

9.1 Major Classes of prn Generators

The earliest, purely deterministic method of generating prn's was the mid-squares method[2)] proposed by von Neumann [7]. We take a number x_n that has $2a$ digits and square it. The resulting product has $4a$ digits, of which the a most significant and the a least significant digits are discarded. Then x_{i+1} is formed from the remaining $2a$ digits as

$$x_{i+1} = \left[\frac{x_i^2}{b^a}\right] - \left[\frac{x_i^2}{b^{3a}}\right] \cdot b^{2a}, \tag{9.2}$$

where b is the base of the number representation. This method of generating prn's was soon abandoned since it degenerates into a cyclic one, often with a very short period. In the worst case, the period comprises just one number.

9.1.1 Linear Recurrence Methods

Many of the prn generators now in use are special cases of the relation

$$x_{i+1} \equiv a_0 x_i + a_1 x_{i-1} + \cdots + a_j x_{i-j} + b \pmod{P}. \tag{9.3}$$

One initiates the generator by starting with a vector of $j+1$ numbers $x_0, x_1, \ldots, x_j$. The generators are characterized by a period τ, which in the best case cannot exceed $P^{j+1} - 1$. The length of τ and the statistical properties of the prn sequences depend on the values of the a_j, b, and P.

Multiplicative Congruential Generators

With the choice of $a_j = 0$, $j \geq 1$, and $b = 0$, one has the multiplicative congruential generator (MCG) introduced by Lehmer [8],

$$x_{i+1} \equiv \lambda \cdot x_i \pmod{P}. \tag{9.4}$$

Only one value of x, x_0, called the *seed*, is needed to begin the recursion. Each value of x_i is scaled into the interval $(0, 1)$ by dividing by P,

$$\xi_i = x_i / P.$$

To obtain the maximum period, $\tau = P - 1$, for the full sequence, the parameters λ and P must be chosen to satisfy certain criteria [9]. When first introduced, P was usually chosen to be a power of 2, especially 2^β where β was the word length on the computer used. However, in this case, the maximum period is reduced to $2^{\beta-2}$ and is only achieved if $\lambda \equiv \pm 3 \pmod 8$. In general, the recursion in Equation 9.4 will begin to repeat after k steps, where $\lambda^k \equiv 1 \pmod P$. The maximum period will

2) For a historical antecedent of this method from the thirteenth century, see chapter 1 of [6].

be achieved when λ and P are relatively prime (no factors in common) and λ is a primitive root modulo P.

But in addition to a large period, we want our generator to produce sequences of prn that are indistinguishable from truly random sequences in statistical tests. Owing to the extensive work by Niederreiter [4], L'Ecuyer [10] and Fishman and Moore [11], one can tailor the choice of λ (given P) to give acceptable distributions of s-tuples of successive prn's (i.e. vectors $(x_n, x_{n+1}, \ldots, x_{n+s-1})$) in s-dimensional space. In a famous paper, Marsaglia [12] showed that the multiplicative congruential generators then in use gave very poor distributions of s-tuples; i.e. the s-tuples lie on a maximum of $(s!P)^{1/k}$ equidistant, parallel hyperplanes within the s-dimensional hypercube $(0, 1)^s$. He questioned the use of such generators in serious Monte Carlo work. Following the advice cited above, recommended values for the parameters λ and P will give reasonable statistical properties in many-dimensional spaces; however, the limitation is the length of the period.

If the parameter b in Equation 9.4 is not set equal to 0, then we have the mixed congruential generator

$$x_{i+1} \equiv \lambda x_i + b \pmod{P}. \tag{9.5}$$

The exact value of the increment b, provided that it is nonzero, has very little influence on the behavior of the generator; the statistical properties are mostly governed by the choice of λ and P.

Multiple Recursive Generators

In multiple recursive generators (MRGs), $j > 0$ in Equation 9.3, so they can achieve much larger periods than MCGs. Computational efficiency is enhanced if some of the a_j are chosen to be 0 or 1. Using criteria developed by Knuth [3], if $a_1 = 1$, the other a_j can be chosen to yield the maximum period. However, limiting the nonzero coefficients to only two can lead to a bad distribution of s-tuples [13]. Examples of good choices for the a_j for a given value of P have been suggested [14–16]. As mentioned previously, the MRG needs to be seeded with $j + 1$ initial values.

A variation of the MRG is the ''multiply-with-carry'' generator introduced by Marsaglia and Zaman [17],

$$x_{i+1} \equiv \lambda x_i + c_i \pmod{P}. \tag{9.6}$$

Here, $c_1 = 0$, $c_{i+1} = 0$ if $x_i + c_i < P$, otherwise, $c_{i+1} = 1$. The generator was generalized with more terms in [18, 19] and recommendations for specific parameters were given. It was shown that the sequences produced by the ''multiply-with-carry'' and its generalizations are identical to those generated by an MCG.

Lagged Fibonacci Congruential Generators

These generators are a generalization of a simple Fibonacci sequence, $x_{i+2} = x_{i+1} + x_i$, and use the recursion,

$$x_i \equiv x_{i-\ell} + x_{i-m} \pmod{P}. \tag{9.7}$$

Here, the a_j of Equation 9.3 are either 0 or 1. If P is prime and $m > \ell$, then the maximum period is $P^m - 1$. However, if $P = 2^\beta$, the maximum period that can be achieved is reduced to $(2^m - 1)2^{\beta-1}$. Also, in the worst case, the lattice structure of 3-tuples are constrained to two planes [20]. To avoid this problem, some of the numbers in a sequence can be discarded to disband bad vectors [3]. For example, ℓ successive values from Equation 9.3 are used and then the next m values are discarded, where $m > \ell$.

9.1.2 Tausworthe or Feedback Shift Register Generators

The linear recurrence relation in Equation 9.3 can be used to generate pseudorandom digits in addition to numbers. Tausworthe [21] introduced a method to produce binary digits; that is, $P = 2$. All the coefficients a_j and the resulting bits, b_i, are either 1 or 0:

$$b_i = a_1 b_{i-1} + \cdots + a_j b_{i-j} \pmod 2. \tag{9.8}$$

Each bit b_i is determined by the previous j bits, $(b_{i-1}, \ldots, b_{i-j})$, which can assume a maximum of 2^j values. If all the j bits are 0, then all future b_i will be 0 and must be avoided . Therefore, the maximum possible period is $2^j - 1$.

The recursion in Equation 9.8 is associated with the primitive polynomial

$$f(\gamma) = a_j + a_{j-1}\gamma + a_{j-2}\gamma^2 + \cdots + a_1\gamma^{j-1} + \gamma^j. \tag{9.9}$$

To determine whether the maximum period is achieved for a specific choice of the a_j, the factorization of Equation 9.9 over the Galois field of two elements must be investigated. The aim is to identify the values of the a_j (a sequence of 0s and 1s) and j that will give statistical independence of successive terms in sequences.

For reasons of computational efficiency, most proposed Tausworthe generators are based on primitive trinomials [22]. That is,

$$b_i = b_{i-p} \oplus b_{i-(p-q)}, \tag{9.10}$$

where $\oplus$ indicates a bitwise exclusive or (addition without carry). The underlying primitive trinomial is

$$1 + \gamma^p + \gamma^{p-q}, \quad p > q. \tag{9.11}$$

A sequence of Q bits, generated by Equation 9.10, can be interpreted as an integer, y_i, base 2. If Q is relatively prime to $2^j - 1$, then the period of a sequence of Q-tuples will also be $2^j - 1$. Tausworthe suggested that a prn in the interval (0, 1) be formed as

$$\xi_i = \sum_{s=1}^{Q} 2^{-s} b_{id+s} = 0.b_{id+1} \cdots b_{id+Q}, \tag{9.12}$$

where the parameter d is called the *decimation*. If the greatest common denominator of d and $2^j - 1$ is 1, then the ξ have a period of $2^j - 1$. A summary of the theoretical

behavior of Tausworthe generators under various statistical tests has been given by Niederreiter [23] and Tezuka [24]. The recurrence in Equation 9.10 requires that the previous p iterates be stored. Also, the initialization of the Tausworthe generator must be implemented carefully. If the mth and nth bits, $m, n < Q$, are identical in each of the first p integers, then they will remain identical in the whole sequence. Tausworthe generators also suffer from a correlated lattice structure of s-tuples in s-dimensional space [5].

Generalized Feedback Shift Register Generators

A variation of the Tausworthe generator, the generalized feedback shift register (GFSR) generator, introduced a lag between the bits used to create the Q-bit integer,

$$y_i = b_i b_{i-\ell_2} \cdots b_{i-\ell_Q}, \tag{9.13}$$

where the $\ell_2, \ldots, \ell_Q$ represent the lags. Since each bit is still generated by Equation 9.10, the y_i satisfy the recursion

$$y_i = y_{i-p} \oplus y_{i-(p-q)}. \tag{9.14}$$

Pseudorandom numbers are obtained from y_i by

$$\xi_i = 2^{-Q} y_i.$$

The starting values for the recursion, Equation 9.14, need not satisfy Equation 9.13; however, the period is then dependent on the starting values. Recommendations for good choices of p and q are given in Fushimi [25]. GFSR generators based on primitive pentanomials,

$$b_i = b_{i-a} \oplus b_{i-b} \oplus b_{i-c} \oplus b_{i-d},$$

are discussed in [26].

Twisted Generalized Feedback Shift Register Generators

Another variation of the GFSR "twists" the bits in the recurrence equation,

$$y_i = y_{i-p} \oplus A y_{i-(p-q)},$$

where A is a $Q \times Q$ matrix of 1s and 0s. The *twisted* GFSR generators can exhibit very large periods. For example, the generator proposed in [27] has a period of 2^{800} and has passed many stringent tests [28]. However, Tezuka [24] revealed important shortcomings in this generator. A more robust version [29] with a period of $2^{19937} - 1$ has been introduced.

9.1.3 Nonlinear Recursive Generators

As was previously mentioned, most generators based on linear recursion exhibit some type of lattice structure when s-tuples, either consecutive or with lags, are

investigated. This is a serious problem in applications that consume prn's s at a time and are therefore sensitive to s-dimensional correlations. Pseudorandom number generators that rely on a nonlinear recursion become an attractive alternative.

Recursive Inversive Generators

Let the recursion for generating pseudorandom integers be given by Eichenauer and Lehn [30],

$$x_{i+1} \equiv a\overline{x_i} + b \pmod{P}, \tag{9.15}$$

where $\overline{x}$ indicates the multiplicative inverse of x modulo P, $1 \equiv \overline{x}x \bmod (P)$. A prn on $(0, 1)$ is obtained as

$$\xi_i = \frac{x_i}{P}.$$

The behavior of the generator in Equation 9.15 is governed by the choice of $a \neq 0$, b, P, and x_0. The sequence $x_0, x_1, \ldots$ is a purely periodic sequence with period $\tau \leq P$. If a and b are chosen such that $x^2 - bx - a$ is a primitive polynomial over the field of order P, then $\tau = P$. Furthermore, if P is a Mersenne prime[3)], and a and b are chosen such that $\tau = P$, the full sequence will pass all s-dimensional lattice tests for $s \leq P - 2$ [31]. However, a lack of linear correlations does not imply that nonlinear correlations are missing. Furthermore, the cost of doing modular inversion is $O(\log_2 P)$ times the cost of doing multiplication.

9.1.4 Combination Generators

One technique that may improve the properties and period of a prng is to combine two or more independent generators in some interesting way. Marsaglia [32] presented a heuristic argument about the sequences produced by combined generators that asserted they are as nearly uniform as either of the original sequences. Additional heuristic justifications for using such generators are given in [33]. One compelling reason is that the combined generator usually has a much longer period than the component generators. A combined generator may employ several generators of the same type or may use different types to create a ''hybrid.'' An example of the former that uses three MCGs was proposed by Wichmann and Hill [34]. The three short period generators are given by $x_i \equiv 171\ x_{i-1} \pmod{30\,269}$, $y_i \equiv 172\ y_{i-1} \pmod{30\,307}$, and $z_i \equiv 170\ z_{i-1} \pmod{30\,323}$, with the resulting prn given by

$$\xi_i = \frac{x_i}{30\,269} + \frac{y_i}{30\,307} + \frac{z_i}{30\,323} \pmod 1.$$

The period of the combined generator is $\approx 10^{12}$. Analysis of the generator has shown that it is equivalent to a single MCG with multiplier 16 555 425 264 690 and

3) Any number that is prime and can be expressed as $2^n - 1$ is called a *Mersenne prime*.

modulus 27 817 185 604 309 [35]. Thus, it has a well-defined lattice structure and higher-order correlations that compare well with other large moduli MCGs [36].

MRGs may also be combined to create a generator with a larger modulus and longer period. If each individual modulus, P_ℓ, $\ell = 1, \ldots, L$, is prime and each component generator has maximal period length, $\tau_\ell = P_\ell^j - 1$, j is the number of terms in the recursion; the period of the combined generator is $\tau_1 \times \cdots \times \tau_L / 2^{L-1}$ [14]. The coefficients of the individual MRG should be chosen such that the combined generator has a good lattice structure in higher dimensions.

9.2 Statistical Testing of prng's

It is unlikely that any one prng will be appropriate in every application. There are requirements, however, that all good prng's should meet. For example, they should have long periods and good lattice structure in the dimensions where they will be most used. Theoretical tests usually consider the behavior of the full period of the sequence. It is possible for a prng to pass a theoretical test, but to have unacceptable behavior in short subsequences. Therefore, it is necessary to subject sequences of prn's to empirical tests. In particular, tests that mimic the behavior of the system of interest are especially relevant. In the discussion below, some examples of the types of statistical tests used are listed. A more thorough description is given in References [2–4].

9.2.1 Theoretical Tests

The spectral test, introduced by Coveyou and MacPherson [37], determines the hyperplane separation in s dimensions that is present in the full-period sequence produced by MCGs. The test uses Fourier analysis applied to the specific generator equations and the full sequence. The computational effort to complete the spectral test is quadratic in the modulus of the generator and exponential in the number of dimensions, s. The lattice structure can also be investigated by looking for the maximum discrepancy from the expected number, N, of occurrences of s-tuples in subregions of the unit hypercube [4]. This test can be applied to any generator, but is very computationally intensive, $O(N^s)$.

A recently developed test, the empirical spectral test [38], combines aspects of theoretical tests such as the spectral test and the discrepancy measure with empirical testing and can be applied to any sequence of prn's or bits. The empirical probability distribution function is generated over a grid of b intervals per dimension in an s-dimensional hypercube. An s-dimensional discrete Fourier transform is applied and the resulting coefficients compared with those expected from a truly random sequence of numbers. The computational complexity is $O(sb \log_2 b)$ and the test can therefore be applied to very long period generators.

9.2.2 Empirical Tests

Large suites of empirical tests for prng's are currently available; see, for example, those maintained by the National Institute of Standards and Technology [39]. A few representative tests are briefly described below.

Equidistribution Test

The interval $(0, 1)$ is divided into k subintervals. The number N_j of values falling into each subinterval is determined for a sequence of prn's, $x_1, \ldots, x_N$. Then a chi-square test is performed where the expected number in each subinterval is $\frac{N}{k}$. The chi-squared value is then

$$\chi^2 = \frac{k}{N} \sum_{j=1}^{k} \left(N_j - \frac{N}{k} \right)^2 . \tag{9.16}$$

Serial Test

In this test, we check the interdependence between successive prn's in a sequence. We consider sets of points

$$\boldsymbol{x}_n = x_n, x_{n+1}, \ldots, x_{n+s-1}$$

in s-dimensional space, where $s \geq 2$. The space is divided into r^s partitions, and the frequency with which s-tuples fall into each partition is measured for a large sequence of prn's. Truly random numbers are uniformly distributed in the s-dimensional space, so we may compute a χ^2 value for our prn generator as

$$\chi^2 = \frac{r^s}{N} \sum^{r} \left(N_{j_1, \ldots, j_s} - \frac{N}{r^s} \right)^2 , \tag{9.17}$$

where $N_{j_1, \ldots, j_s}$ is the number of s-tuples occuring in partition $(j_1, \ldots, j_s), j_i = 1, \ldots, r$ and $i = 1, \ldots, s$. χ^2 should behave asymptotically as a χ^2 distribution with $r^s - 1$ degrees of freedom.

Runs-up and Runs-down Test

Here we compare the magnitude of a prn with the preceding one. If $x_{n-1} > x_n < x_{n+1} < x_{n+2} > x_{n+3}$, then we say we have a run-up of length 3. In a sequence of prn's, we count the number of run-ups of length 1, length 2, ... For truly random numbers, where each of the x_i is independent of the others and all permutations are equally likely, we expect the number of occurrences of run-ups (or run-downs) of length r to be given by the formula

$$R_r = \frac{(N+1)(r^2 + r - 1) - (r+2)(r^2 - r - 1)}{(r+2)!}. \tag{9.18}$$

N is the total number of samples in the prn sequence. Since adjacent runs are not independent, we cannot apply a χ^2 test directly but must compute a different statistic [3],

$$V = \frac{1}{N} \sum_{1<i,j<t} (\text{Count}(i) - R_i)(\text{Count}(j) - R_j)a_{ij}. \tag{9.19}$$

Count(i) is the actual observed number of run-ups (or run-downs) of length i, and the a_{ij} are the elements of the inverse of the covariance matrix. Once V is computed, it can be compared with a χ^2 distribution of degree t.

The run test is an important one. Congruential generators with multipliers that are too small tend to have runs either much longer or shorter than expected.

9.3 Comparing Two Pseudorandom Number Generators

To illustrate the type of behavior observed when tests are applied to specific prng's, two mixed congruential generators with relatively short periods are subjected to the tests described in Section 9.2.2.

9.3.1 A Multiplicative Congruential Generator Proposed for 32-bit Computers

The first mixed congruential generator considered here was recommended for use on a 32-bit machine as one whose multiplier satisfied spectral tests for pairs of points [40]. However, since the modulus is not prime, the period will be at most 2^{30}, which is quite short. We have

$$\begin{aligned} &\lambda = 1 \text{ and } 812 \text{ and } 433 \text{ and } 253, \\ &P = 2^{32}, \text{and} \\ &b = \text{odd}. \end{aligned} \tag{9.20}$$

For the equidistribution test, Equation 9.20, sequences of 10 000 prn's were placed in 100 bins equispaced on $(0, 1)$. The expected number in each bin is 100, and a χ^2 value was computed. The whole test was repeated 1000 times to generate 1000 values of χ^2, since a single unacceptable χ^2 value is always possible. If the sequence being treated is uniform, then $\chi^2_1, \chi^2_2, \ldots, \chi^2_{1000}$ should behave like a random sample from a $\chi^2(99)$ distribution, and this can be tested by again applying a chi-square test [3]. We sort the values of χ^2_i, $i = 1, \ldots, 1000$ into 100 equally probable intervals $(0, \chi^2(99, 0.01))$, $(\chi^2(99, 0.01), \chi^2(99, 0.02))$, $\ldots$, $(\chi^2(99, 0.98), \chi^2(99, 0.99))$, $(\chi^2(99, 0.99), \chi^2(99, 1.0))$, where the expected number B_i in each interval is 10. Figure 9.1 contains the distribution of χ^2 values obtained. The overall χ-squared value is then

$$\chi^2_T = \sum_{j=1}^{100} \frac{(B_j - 10.)^2}{10.} = 82.2 \tag{9.21}$$

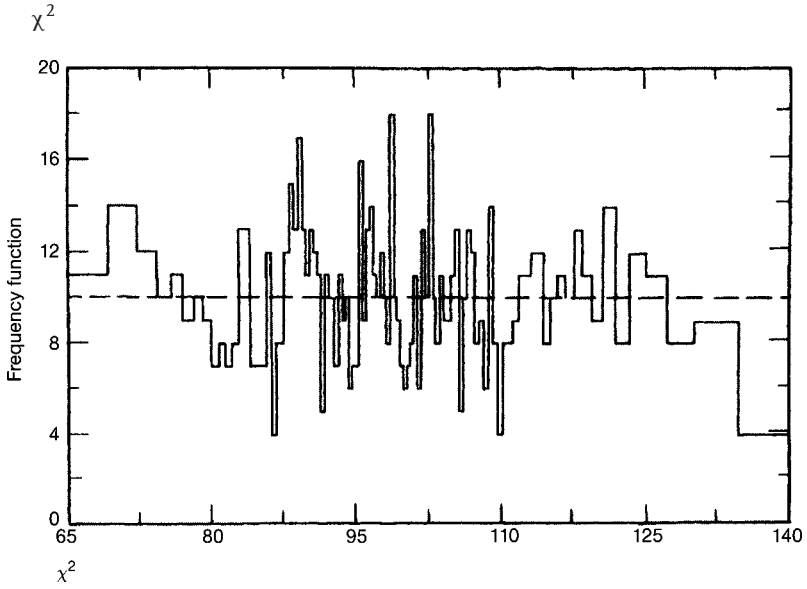


Figure 9.1 The frequency function of observed values of χ^2 after 1000 samples. The bins are equally probable intervals where the expected number of χ^2 in each bin is 10. The pseudorandom number generator was Equation 9.20.

for the random number generator in Equation 9.20. In this case, the smaller the value of χ_T^2, the better the generator. The value of 82.2 is an acceptable value.

The serial test (Section 9.2.2) was performed for $s = 2$; that is, interdependence between pairs of prn's was studied. Sets of 10 000 pairs of prn's were produced and partitioned into a 10×10 array. A typical distribution of the pairs of prn's is shown in Table 9.1 with its associated χ^2 value. Since we have 100 partitions, the expected number of pairs in each partition is 100. As in the equidistribution test above, the whole test was repeated 1000 times to generate 1000 χ^2 values and an overall χ_T^2 value was calculated. In this case, $\chi_T^2 = 104$, which is again a reasonable value for a sample from a $\chi^2(99)$ distribution.

The prng in Equation 9.20 was also exercised by a runs-up test. A record of runs of length 1–5, 6, and greater was produced, and the statistic V in Equation 9.19 was determined. Table 9.2 shows the observed number of runs of length r and the expected number from Equation 9.18. The value of V, 3.48, is to be compared with a $\chi^2(6)$ distribution and is an acceptable value.

Lastly, the mixed congruential generator in Equation 9.20 was used to produce pairs of Gaussian random numbers by the Box–Muller algorithm. Owing to the use of two sequential uniform random numbers and the periodicity of the trigonometric functions, the Box–Muller algorithm is very sensitive to correlations between pairs of prn's. In Figure 9.2, 5000 pairs of points produced by Equation 3.38 are plotted. The behavior appears likely for a Gaussian distribution centered at zero,

Table 9.1 Partitioning of 10 000 pairs of pseudorandom numbers generated by Equation 9.20 into a 10×10 array.

78	83	89	106	98	105	89	84	118	106
98	100	118	83	93	112	l00	102	94	112
97	76	95	94	101	77	105	103	96	110
106	102	123	102	110	88	112	106	111	84
91	98	96	98	107	114	101	112	108	91
83	93	103	97	91	96	98	89	118	98
89	104	101	116	111	104	105	108	101	95
92	107	95	96	90	106	110	101	106	90
106	100	100	85	102	85	104	112	93	97
91	118	109	114	96	88	119	112	110	84

$\chi^2 = 105.2$

Table 9.2 Observed number of runs of length r compared with the expected number after 10 000 samples for pseudorandom number generator 9.20.

Length of run	Observed	Expected[a]
1	1661	1667
2	2068	2083
3	889	916
4	289	263
5	60	58
6 and over	13	12
	$V = 3.48$	

[a]Calculated using Equation 9.18.

though no values outside the bounds $(-4.0,4.0)$ were sampled. This is reasonable since $\pm\sqrt{-2\log(\nu)}$ are the largest and smallest values that can be produced by the Box–Muller algorithm, where ν is the smallest floating-point number that can be produced by the prng.

From the few tests applied to the prng in Equation 9.20, it appears that in calculations where one or a pair of prn's are needed at a time, Equation 9.20 is an adequate source.

9.3.2
A Bad Random Number Generator

Now that an example of a reasonable prng with a short period has been analyzed, the behavior of a bad one will be contrasted with it. The second mixed congruential

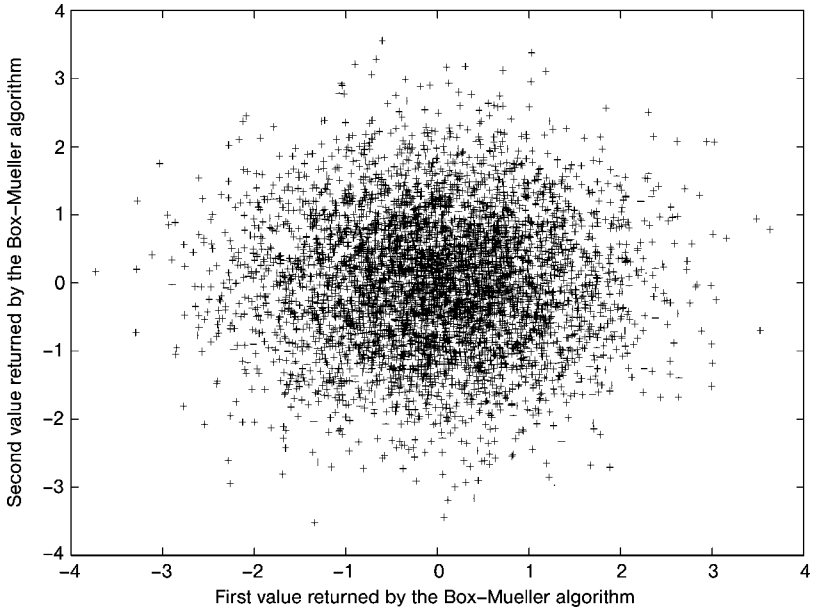


Figure 9.2 Plotting the two Gaussian random variables produced by the Box–Muller algorithm using Equation 9.20 against each other.

generator [3] has the following constants:

$$\lambda = 2^{18} + 1, x_0 = 314159265, \qquad (9.22)$$
$$P = 2^{35}, b = 1,$$

where x_0 is the initial seed. It has an apparently longer period than that of the generator in Equation 9.20. However, the multiplier has not been chosen to satisfy any theoretical criteria.

As in the development given above, Equation 9.22 was subjected to the equidistribution test repeated 1000 times with different sequences and χ_T^2 was determined. Figure 9.3 shows the distribution of the values of χ^2, which is seen to be skewed toward higher values. This is reflected in the value for χ_T^2, which is 1022.0, an unacceptably high value.

The poor behavior of generator 9.22 with the equidistribution test becomes worse in the serial test. Again, pairs of prn's were partitioned into a 10×10 array. A typical example of a partitioning of 10 000 pairs is shown in Table 9.3, where the pairs of prn's are clearly not uniformly distributed. The value for χ_T^2 associated with 1000 repetitions of the test was 99 999.

The generator 9.22 fares no better with the runs test. As shown in Table 9.4, the distribution of run-ups of length r does not resemble the expected distribution given by 9.18.

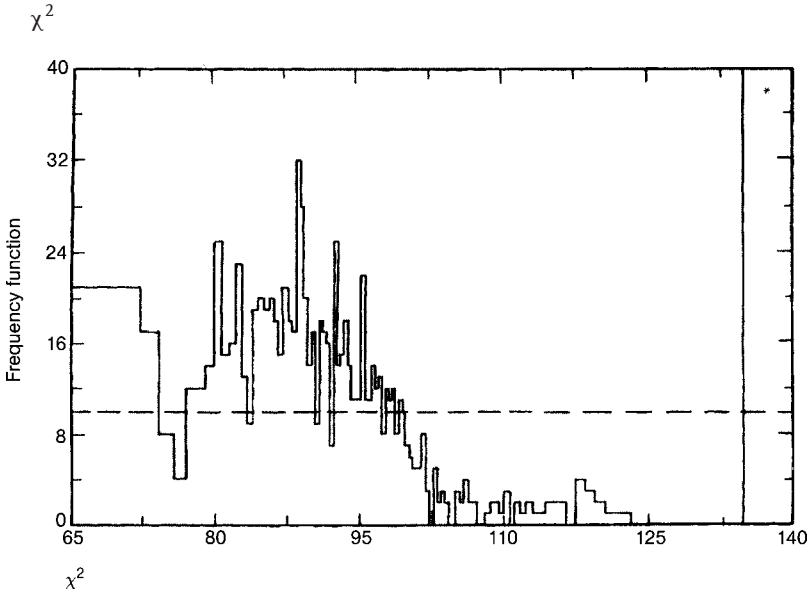


Figure 9.3 The frequency function of observed values of χ^2 after 1000 samples using prn generator Equation 9.22. The expected number of χ^2 in each bin is 10. The value of the bin indicated by $*$ is off scale.

Table 9.3 Partitioning of 10 000 pairs of pseudorandom numbers generated by Equation 9.22 into a 10×10 array.

332	0	0	0	0	0	0	0	99	577
575	311	0	0	0	0	0	0	0	99
99	557	304	0	0	0	0	0	0	0
0	131	574	308	0	0	0	0	0	0
0	0	106	580	314	0	0	0	0	0
0	0	0	105	609	314	0	0	0	0
0	0	0	0	100	589	315	0	0	0
0	0	0	0	0	91	585	321	0	0
0	0	0	0	0	0	112	579	319	0
0	0	0	0	0	0	0	108	573	314

$\chi^2 = 34\,686$

Finally, 5000 pairs of Gaussian variables were sampled using the Box–Muller algorithm and plotted in Figure 9.4. A startling amount of correlation is apparent. Also, the sampled values are skewed in their distribution and not sampled symmetrically about zero.

The results of the three tests and the output from using the prng in the Box–Muller algorithm shown here would encourage us not to use generator 9.22 in our Monte Carlo calculations.

Table 9.4 Observed number of runs of length r compared with the expected number after 10 000 samples for pseudorandom number generator 9.22.

Length of run	Observed	Expected[a]
1	7664	1667
2	1168	2083
3	0	916
4	0	263
5	0	58
6 and over	0	12
	$V = 28370$	

[a]Calculated using Equation 9.18.

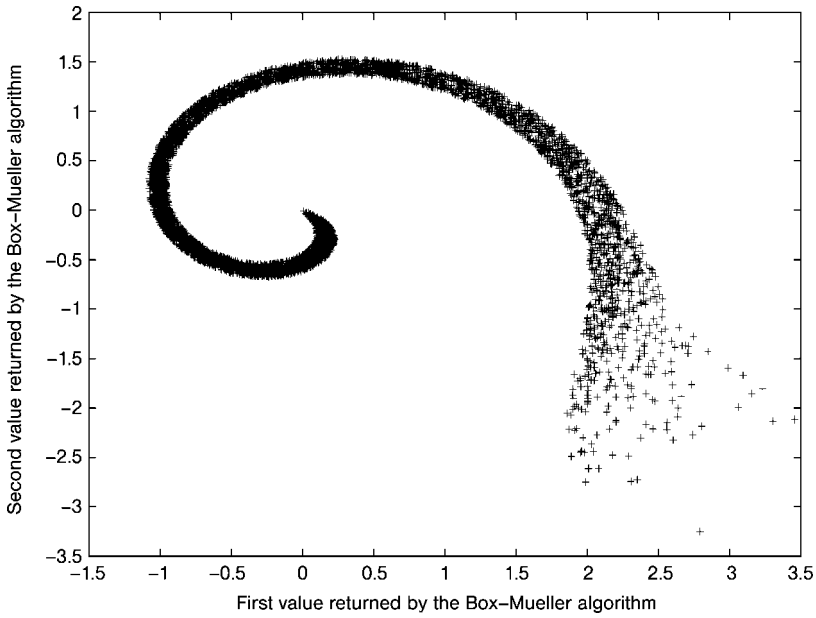


Figure 9.4 Plotting the two Gaussian random variables produced by the Box–Muller algorithm using Equation 9.22 against each other.

9.4 Pseudorandom Number Generation on Parallel Computers

Computations on parallel processors, distributed networks, and clusters of computers pose new and distinctive problems for prng's. Currently, large simulations can consume billions of prn's in the course of a single calculation and thus need

very long pseudorandom sequences. When multiple realizations of a calculation are performed, it is necessary to have readily available multiple, independent sequences. Since large-scale networks may have tens of thousands of processors, it is a challenge to provide enough pseudorandom sequences that predictably reduce the variance by the number of distinct realizations of the calculation. Furthermore, it remains highly desirable that individual runs be reproducible. The difficulty is that on multiple-instruction-stream–multiple-datastream (MIMD) machines, or on distributed networks or clusters, the order in which operations are done and the identity of the processor that carries out a specific task are not necessarily the same when a calculation is repeated. Neither a centralized prng nor even a separate one for each physical processor will guarantee reproducibility.

9.4.1 Splitting and Leapfrogging

The first of the problems cited above can be solved by the use of sequences with very long periods such as a ''twisted'' GFSR generator or a combination generator. In the technique referred to as *splitting*, if n parallel Monte Carlo realizations are being carried out simultaneously and one assigns each realization in advance to use a separate but equal portion of the original sequence, then the length of the subsequence for each is τ/n, where τ is the period of the full sequence. This procedure requires a long-period generator and testing that there are no correlations between the subsequences that would adversely affect the Monte Carlo calculation. It has also been proposed that the starting seeds for parallel subsequences from a single prng be chosen randomly. This approach was analyzed for congruential generators by Zhong and Kalos [41]. It was proved that the probability for no overlap between the randomly chosen parallel subsequences was

$$P\{\text{no overlap}\} = 1 - n\left(\frac{m}{\tau}\right)^{n-1},$$

where n is the number of parallel subsequences and m is the number of prn's in each subsequence. The probability becomes 0 very quickly even for modest values of n and m.

In another approach, called *leapfrogging*, a new sequence is created from the original one by skipping numbers in a predetermined pattern, e.g. $x_r, x_{r+k}, x_{r+2k}, \ldots$. The next sequence could begin at x_{r+1}, with the same value for k. If the skipping distance is relatively prime with respect to the period, the new sequence will have the same period as the original. The correlation between the sequences $(x_i, \ldots)$ and $(x_{i+k}, \ldots)$ for MCGs has been investigated [42]. If $x_{i+k} = (n_1/n_2)x_i$, where n_1 and n_2 are relatively prime, then the correlation is given asymptotically by $1/(n_1 n_2)$.

9.4.2 Parallel Sequences from Combination Generators

Combination generators offer another method of providing parallel sequences of prn's. One proposal [43] was a hybrid combination generator that used an MCG

with a lagged Fibonacci generator. To provide k sequences in total, the jth sequence, $j = 1, \ldots, k$, is given by

$$x_{j,i} = a^k x_{j,i-1} \pmod{P},$$
$$v_{j,i} = \frac{x_{j,i}}{P},$$
$$y_{j,i} = f(y_{j,i-1}, \ldots), \textit{and}$$
$$\xi_{j,i} = (v_{j,i} - y_{j,i}) \pmod{P},$$

where the initial seed for each sequence is $a^j x_0$. The sequences do not overlap, but exhibit the lattice structure of congruential generators.

Another approach [44] developed a method of generating independent sequences of prn's based on a generalization of the Wichmann–Hill combination generator [34]. A single generator with d terms is defined as

$$\xi_i = \frac{\sum_{\ell=1}^{d} (a_\ell)^i (\hat{P}/P_\ell) x_{\ell,0} \pmod{\hat{P}}}{\hat{P}}, \tag{9.23}$$

where $\hat{P} = \prod P_\ell$, $\ell = 1, \ldots, d$, all the d moduli are coprime, and the a_ℓ are selected to give a full period. To produce k parallel sequences based on Equation 9.23, let $j = 1, \ldots, k$,

$$\xi_{j,i} = \frac{A_{j,i} \pmod{\hat{P}_j}}{\hat{P}_j},$$

with

$$\hat{P}_j = \prod_{\ell=1}^{d} P_{\ell j} \text{ and}$$
$$A_{j,i} = \sum_{\ell=1}^{d} (a_{\ell j})^i \frac{\hat{P}_j}{P_{\ell j}} x_{\ell j,0},$$

where the $(x_{1,j,0}, \ldots, x_{d,j,0})$ are the seeds for the jth sequence. With the requirement that all the moduli must be coprime, it is straightforward to make available several thousand parallel sequences with periods of at least 2^{80}. The statistical independence of the sequences was tested by a parallel spectral test [44] and shown to be on the order of $1/\hat{P}_j$.

9.4.3 Reproducibility and Lehmer Trees

Reproducibility of Monte Carlo runs is, in principle, easy to ensure. It is simply necessary that each initialization of a parallel task such as a new random walk or the "spawning" of a daughter walker (as in a branching or multiplying system) be

given an independent prn sequence. Zhong and Kalos [41] and Fredrickson *et al.* [45] introduced the concept of a pseudorandom tree, in which one generator is used for ''intraprocess'' random numbers, and a separate one for initialization. This was called a *Lehmer tree*. Fredrickson *et al.* [45] proved a necessary condition for nonoverlapping of the resulting sequences when mixed congruential generators were used. The Lehmer tree algorithm was generalized by Percus and Kalos [46] such that each sequence differed from the others by use of a different additive constant in Equation 9.5,

$$x_{L,j} = a_L x_{L,j-1} + b_L \pmod{P}, \tag{9.24a}$$

$$x_{j,i} = a_R x_{j,i-1} + b_j \pmod{P}. \tag{9.24b}$$

The generator in Equation 9.24a is used solely to provide seeds for the jth sequence given by Equation 9.24b, where $j = 1, \ldots, k$. The differing values of b_j guarantee that each sequence is reordered and no overlapping sequences occur. In addition, Percus and Kalos developed a spectral test for k parallel mixed congruential generators to measure the uniformity of points in k-dimensional space. Recommendations were given for choosing the b_j's, $j = 1, \ldots, k$ such that all $\binom{k}{2}$ pairs of a k-component random vector satisfy the spectral test.

9.4.4
SPRNG: A Library of Pseudorandom Number Generators

The concept of giving each parallel task its own generator while minimizing the correlations between the parallel sequences has lead to the development of the SPRNG software library [47]. The library incorporates the ideas of previous researchers though the use of an indexed binary tree of prng's. The types of prng's included in the library are parameterized families of MCGs, lagged Fibonacci generators, and combined MRGs. Reproducibility of a parallel calculation is guaranteed by the indices of the binary tree and the seed values of the generators. The software library may be used on both parallel computers and distributed networks.

9.5
Summary

In choosing the source of prn's for their simulation, researchers should be aware of both the strengths and the weaknesses of the selected generator. The prng should show uniformity in the number of dimensions important to the simulation, it should not exhibit correlations that will adversely affect the calculation, it should have a long enough period that only a small subset of the period will be consumed in any single realization, and it should be fast enough that the generation of uniform pseudorandom variables does not dominate the computational time. It is unlikely that any one prng will satisfy the criteria for every calculation. The best approach is to have a suite of different types of prng's available for use in both testing and production calculations.

References

1 Kac, M. (**1983**) What is random? *American Scientist*, **71**, 405.

2 Gentle, J.E. (**2003**) *Random Number Generation and Monte Carlo Methods*, 2nd edn, Springer-Verlag, New York, Berlin, Heidelberg.

3 Knuth, D.E. (**1998**) *The Art of Computer Programming, Semi-Numerical Algorithm*, Vol. 2, 3rd edn, Addison-Wesley, Reading, MA.

4 Niederreiter, H. (**1992**) *Random Number Generation and Quasi-Monte Carlo Methods*, Society for Industrial and Applied Mathematics, Philadelphia, PA.

5 Ripley, B.D. (**1987**) *Stochastic Simulation*, John Wiley & Sons, Ltd, New York.

6 Ekeland, I. (**1993**) *The Broken Dice and Other Mathematical Tales of Chance*, The University of Chicago Press, Chicago, IL; translated by Carol Volk.

7 von Neumann, J. (**1951**) Various techniques used in connection with random digits, *NBS Applied Mathematics Series*, Vol. 12, U.S. Government Printing Office, Washington, DC, pp. 36–38.

8 Lehmer, D.H. (**1951**) Mathematical methods in large-scale computing units. *Annals of the Computation Laboratory of Harvard University*, **26**, 141.

9 Jansson, B. (**1966**) *Random Number Generators*, Almquist and Wiksell, Stockholm.

10 L'Ecuyer, P. (**1988**) Efficient and portable combined random number generators. *Communications of the ACM*, **31**, 742.

11 Fishman, G.S. and Moore, L.R. (**1986**) An exhaustive analysis of multiplicative congruential random number generators with modulus $2^{31} - 1$. *SIAM Journal on Scientific and Statistical Computing*, **7**, 24.

12 Marsaglia, G. (**1968**) Random numbers fall mainly in the planes. *Proceedings of the National Academy of Sciences of the United States of America*, **61**, 25.

13 L'Ecuyer, P. and Touzin, R. (**2004**) On the Deng-Lin random number generators and related methods. *Statistics and Computing*, **14**, 5.

14 L'Ecuyer, P. (**1999**) Good parameters and implementations for combined multiple recursive random number generators. *Operations Research*, **47**, 159.

15 Kao, C. and Tang, H.C. (**1997**) Systematic searches for good multiple recursive random number generators. *Computers and Operations Research*, **24**, 899.

16 Deng, L.-Y. and Xu, X. (**2003**) A system of high-dimensional, efficient, long-cycle and portable uniform random number generators. *ACM Transactions on Modeling and Computer Simulation*, **13**, 299.

17 Marsaglia, G. and Zaman, A. (**1991**) A new class of random number generators. *The Annals of Applied Probability*, **1**, 462.

18 Couture, R. and L'Ecuyer, P. (**1997**) Distribution properties of multiply-with-carry random number generators. *Mathematics of Computation*, **66**, 591.

19 Goresky, M. and Klapper, A. (**2003**) Efficient multiply-with-carry random number generators with maximal period. *ACM Transactions on Modeling and Computer Simulation*, **13**, 310.

20 L'Ecuyer, P. (**2004**) Random number generation, in *Handbook of Computational Statistics* (eds J.E. Gentle, W. Haerdle and Y. Mori), Springer-Verlag, Berlin.

21 Tausworthe, R.C. (**1965**) Random numbers generated by linear recurrence modulo two. *Mathematics of Computation*, **19**, 201.

22 Kumada, T., Leeb, H., Kurita, Y. *et al.* (**2000**) New primitive t-nomials ($t = 3, 5$) over GF(2) whose degree is a Mersenne exponent. *Mathematics of Computation*, **69**, 811.

23 Niederreiter, H. (**1982**) Statistical tests for Tausworthe pseudo-random numbers, in *Probability and Statistical Inference* (eds W. Grossmann, G.C. Pflug and W. Wertz), Reidel, Dordrecht.

24 Tezuka, S. (**1995**) *Uniform Random Numbers: Theory and Practice*, Kluwer Academic Publishers, Norwell, MA.

25 Fushimi, M. (**1990**) Random number generation with the recursion $X_t = X_{t-3p} \oplus X_{t-3q}$. *Journal of Computational and Applied Mathematics*, **31**, 105.

26 Ziff, R.M. (**1998**) Four-tap shift-register-sequence random-number generators. *Computers in Physics*, **12**, 385.

27 Matsumoto, M. and Kurita, Y. (**1994**) Twisted GFSR generators II. *ACM Transactions on Modeling and Computer Simulation*, **4**, 245.

28 Hellekalek, P. (**1998**) Good random number generators are (not so) easy to find. *Mathematics and Computers in Simulation*, **46**, 485.

29 Matsumoto, M. and Nishimura, T. (**1998**) Mersenne twister: a 623-dimensionally equidistributed uniform pseudo-random number generator. *ACM Transactions on Modeling and Computer Simulation*, **8**, 3.

30 Eichenauer, J. and Lehn, J. (**1986**) A non-linear congruential pseudo-random number generator. *Statistische Hefte*, **27**, 315.

31 Chou, W.-S. and Niederreiter, H. (**1995**) On the lattice test for inversive congruential pseudo-random numbers, in *Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing* (eds H. Niederreiter and P.J.-S. Shiue), Springer-Verlag, New York, pp. 186.

32 Marsaglia, G. (**1985**) A current view of random number generators, in *Computing Science and Statistics, 16th Symposium on the Interface* (ed L. Billard), North-Holland, Amsterdam.

33 Deng, L.-Y. and George, E.O. (**1990**) Generation of uniform variates from several nearly uniformly distributed variables. *Communications in Statistics - Simulation and Computation*, **19**, 145.

34 Wichmann, B.A. and Hill, I.D. (**1982**) Algorithm AS183: an efficient and portable pseudo-random number generator. *Applied Statistics*, **31**, 188.

35 Ziesel, H. (**1986**) A remark on Algorithm AS183: an efficient and portable pseudo-random number generator. *Applied Statistics*, **35**, 89.

36 De Matteis, A. and Pagnutti, S. (**1993**) Long-range correlation analysis of the Wichmann-Hill random number generator. *Statistics and Computing*, **3**, 67.

37 Coveyou, R.R. and MacPherson, R.D. (**1967**) Fourier analysis of uniform random number generators. *Journal of the ACM*, **14**, 100.

38 Zeitler, D., McKean, J. and Kapenga, J. (**2002**) Empirical spectral analysis of random number generators. *Computing Science and Statistics*, **34**, 157.

39 http://www.csrc.nist.gov/groups/ST/toolkit/rng/index.html.

40 Borosh, I. and Niederreiter, H. (**1983**) Optimal multipliers for pseudo-random number generations by the linear congruential method. *Behaviour and Information Technology*, **23**, 65.

41 Zhong, Y.-Q. and Kalos, M.H. (**1983**) *Monte Carlo Transport Calculations on an Ultracomputer*, Ultracomputer Note # 46, CIMS, New York University, New York.

42 Anderson, N.H. and Titterington, D.M. (**1993**) Cross-correlation between simultaneously generated sequences of pseudo-random uniform deviates. *Statistics and Computing*, **3**, 61.

43 Wollan, P.C. (**1992**) A portable random number generator for parallel computers. *Communications in Statistics – Simulation and Computation*, **21**, 1247.

44 Maclaren, N.M. (**1989**) The generation of multiple independent sequences of pseudo-random numbers. *Applied Statistics*, **38**, 351.

45 Fredrickson, P., Hiromoto, R., Jordan, T.L. *et al.* (**1984**) Pseudo-random trees in Monte Carlo. *Parallel Computing*, **1**, 175.

46 Percus, O.E. and Kalos, M.H. (**1989**) Random number generators for MIMD parallel processors. *Journal of Parallel and Distributed Computing*, **6**, 477.

47 Mascagni, M. and Srinivasan, A. (**2000**) SPRNG: a scalable library for pseudo-random number generation. *ACM Transactions on Mathematical Software*, **26**, 346.

Index

Monte Carlo Methods. Second Edition. M.H. Kalos and P.A. Whitlock

ISBN: 978-3-527-40760-6