

2

SOME PROBABILITY AND STATISTICS REVISION

We have seen from Chapter 1 that in many uses of simulation, statisticians need to simulate discrete and continuous random variables of different kinds, and techniques for doing this are provided in Chapters 4 and 5. The aim of this chapter is to specify what we mean by random variables, and generally to provide revision of the material to be used later.

It will be assumed that the reader is familiar with the axioms of probability and the ideas of independence, and conditional probability. The material assumed is covered in, for example, chapters 1-6 of *ABC*. In the following we shall write $\Pr(A)$ for the probability of any event A . We shall begin with general definitions, and then proceed to consider particular important cases.

2.1 Random variables

Underlying all statistical investigations is the concept of a random experiment, such as the tossing of a coin k times. The set of all possible outcomes to such an experiment is called the *sample-space*, introduced by von Mises in 1921 (he called it a *Merkmalraum*), and we can formally define random variables as functions over the sample-space, about which it is possible to make probability statements. In the simple model of a queue given in Exercise 1.4, the change in queue size forms a random experiment, with just two possible outcomes, namely, an arrival or a departure. With this random experiment we can associate a random variable, X , say, such that $X = +1$ if we have an arrival, and $X = -1$ if we have a departure. The model is such that $\Pr(X = +1) = p$, and $\Pr(X = -1) = 1 - p$. In detail here, the sample-space contains just two outcomes, say ω_1 and ω_2 , corresponding to arrival and departure, respectively, and we can write the random variable X as $X(\omega)$, so that $X(\omega_1) = +1$ and $X(\omega_2) = -1$. However, we find it more convenient to suppress the argument of $X(\omega)$, and

2.3 The probability density function (p.d.f.)

simply write the random variable as X in this example. We shall adopt the now standard practice of using capital letters for random variables, and small letters for values they may take. When a random variable X is simulated n times then we obtain a succession of values: $\{x_1, x_2, \dots, x_n\}$, each of which provides us with a *realization* of X .

Another random experiment results if we record the queue size in the model of Exercise 1.4. From Section 1.6 we see that if $p < \frac{1}{2}$, then after a long period of time since the start of the queueing system we can denote the queue size by a random variable, Y , say, such that Y may take any non-negative integral value, and $\Pr(Y = k)$ for $k \geq 0$ is as given in Section 1.6.

2.2 The cumulative distribution function (c.d.f.)

For any random variable X , the function F , given by $F(x) = \Pr(X \leq x)$ is called the *cumulative distribution function* of X . We have

$$\lim_{x \rightarrow -\infty} F(x) = 0; \quad \lim_{x \rightarrow \infty} F(x) = 1$$

$F(x)$ is a nondecreasing function of x , and $F(x)$ is continuous from the right (i.e. if $x > x_0$, $\lim_{x \rightarrow x_0} F(x) = F(x_0)$).

The nature of $F(x)$ determines the type of random variable in question, and we shall normally specify random variables by defining their *distribution*, which in turn provides us with $F(x)$. If $F(x)$ is a step function we say that X is a *discrete* random variable, while if $F(x)$ is a continuous function of x then we say that X is a *continuous* random variable. Certain variables, called *mixed* random variables, may be expressed in terms of both discrete and continuous random variables, as is the case of the waiting-time experienced by cars approaching traffic lights; with a certain probability the lights are green, and the waiting-time may then be zero, but otherwise if the lights are red the waiting-time may be described by a continuous random variable. Mixed random variables are easily dealt with and we shall not consider them further here. Examples of many common c.d.f.'s are given later.

2.3 The probability density function (p.d.f.)

When $F(x)$ is a continuous function of x , with a continuous first derivative, then $f(x) = dF(x)/dx$ is called the *probability density function* of the (continuous) random variable X . If $F(x)$ is continuous but has a first derivative that is not continuous at a finite number of points, then we can still define the probability density function as above, but for uniqueness we

set $f(x) = 0$, for instance, when $dF(x)/dx$ does not exist; an example of this is provided by the c.d.f. of the random variable Y of Exercise 2.25.

The p.d.f. has the following properties:

- (i) $f(x) \geq 0$
 (ii) $\int_{-\infty}^{\infty} f(x) dx = 1$
 (iii) $\Pr(a < X < b) = \Pr(a \leq X < b) = \Pr(a < X \leq b) = \Pr(a \leq X \leq b)$
 $= \int_a^b f(t) dt$

EXAMPLE 2.1

Under what conditions on the constants α, β, γ can the following functions be a p.d.f.?

$$g(x) = \begin{cases} e^{-\alpha x}(\beta + \gamma x) & \text{for } x \geq 0 \\ 0 & \text{for } x < 0 \end{cases}$$

We must verify that $g(x)$ is non-negative, and that $\int_{-\infty}^{\infty} g(x) dx = 1$. If $\alpha \leq 0$, this integral cannot be finite, and so we must have $\alpha > 0$.

$$\int_{-\infty}^{\infty} g(x) dx = \int_{-\infty}^{\infty} e^{-\alpha x}(\beta + \gamma x) dx = \frac{\beta}{\alpha} + \frac{\gamma}{\alpha^2} \quad \text{OK}$$

Thus we must have $\gamma = \alpha^2 - \alpha\beta = \alpha(\alpha - \beta)$ resulting in the p.d.f.

$$g(x) = e^{-\alpha x}(\beta + \alpha(\alpha - \beta)x) \quad \text{for } x \geq 0$$

In order that $g(x) \geq 0$ for $x \geq 0$, we must have $\beta \geq 0$, and $\alpha \geq \beta$. Hence set $\beta = \theta\alpha$ and $\gamma = \alpha^2(1 - \theta)$, for $\alpha > 0$ and $0 \leq \theta \leq 1$.

We sometimes abbreviate 'probability density function' to just 'density'.

2.4 Joint, marginal and conditional distributions

In the case of two random variables X and Y we can define the joint c.d.f. by $F(x, y) = \Pr(X \leq x \text{ and } Y \leq y)$, and then the univariate distributions of X and Y are referred to as the marginal distributions. If

$$f(x, y) = \frac{\partial^2 F(x, y)}{\partial x \partial y}$$

is a continuous function, except possibly at a finite number of points, then $f(x, y)$ is called the joint p.d.f. of X and Y , and in this case the marginal p.d.f.'s are given by:

$$f_X(x) = \int_{-\infty}^{\infty} f(x, y) dy$$

2.5 Expectation

and

$$f_Y(y) = \int_{-\infty}^{\infty} f(x, y) dx$$

Here we have adopted a notation we shall employ regularly, of subscripting the p.d.f. of a random variable with the random variable itself, so that there should be no confusion as to which random variable is being described. The same approach is adopted for c.d.f.'s, and, also, sometimes, for joint distributions.

The conditional p.d.f. of the random variable Y , given the random variable X , may be written as $f_{Y|X}(y|x)$, and is defined by

$$f_{Y|X}(y|x) = f_{X,Y}(x, y)/f_X(x) \quad \text{if } f_X(x) > 0$$

For two independent continuous random variables X and Y , with joint p.d.f. $f_{X,Y}(x, y)$, we have

$$f_{X,Y}(x, y) = f_X(x) f_Y(y) \quad \text{for any } x \text{ and } y$$

The above definitions of independence and joint, marginal and conditional p.d.f.'s have straightforward analogues for discrete random variables. For example, the marginal distribution of a discrete random variable X may be given by:

$$\Pr(X = x) = \sum_y \Pr(X = x, Y = y)$$

Furthermore, while we have only discussed the bivariate case, these definitions may be extended in a natural way to the case of more than two random variables.

2.5 Expectation

The expectation of a random variable X exists only if the defining sum or integral converges absolutely. If X is a continuous random variable we define the expectation of X as:

$$\mathcal{E}[X] = \int_{-\infty}^{\infty} x f(x) dx \quad \text{if } \int_{-\infty}^{\infty} |x| f(x) dx < \infty$$

where $f(x)$ is the p.d.f. of X . Similarly, if X is a discrete random variable which may take the values $\{x_i\}$, then

$$\mathcal{E}[X] = \sum_i x_i \Pr(X = x_i) \quad \text{if } \sum_i |x_i| \Pr(X = x_i) < \infty$$

The variance of a random variable X is defined as

$$\text{Var}(X) = \mathcal{E}[(X - \mathcal{E}[X])^2]$$

and the covariance between random variables X and Y is defined as

$$\text{Cov}(X, Y) = \mathcal{E}[(X - \mathcal{E}[X])(Y - \mathcal{E}[Y])]$$

The expectation of a random variable X is frequently used as a measure of location of the distribution of X , while the variance provides a measure of spread of the distribution. Independent random variables have zero covariance, but in general the converse is not true.

The correlation between random variables X and Y is defined as

$$\text{Corr}(X, Y) = \frac{\text{Cov}(X, Y)}{\sqrt{[\text{Var}(X) \text{Var}(Y)]}}$$

2.6 The geometric, binomial and negative-binomial distributions

Consider a succession of independent experiments, such as tosses of a coin; at each of which either 'success' (which we could identify with 'heads' in the case of the coin) or 'failure' ('tails' for the coin) occurs. This rudimentary succession of experiments, or trials, provides the framework for three important discrete distributions.

$$\text{Let } p = \text{Pr}(\text{success}) \quad \text{and} \quad q = 1 - p = \text{Pr}(\text{failure})$$

The simplest is the geometric distribution, which results if we let X be the discrete random variable measuring the number of trials until the first success. We have

Geometric distribution:
 $\text{Pr}(X = i) = q^{i-1} p \quad \text{for} \quad 1 \leq i < \infty$

$$\mathcal{E}[X] = 1/p \quad \text{and} \quad \text{Var}(X) = q/p^2 \quad \text{v. c.k.}$$

Figure 2.1(a) gives a bar-chart illustrating the geometric distribution for the case $p = 0.5$. Figure 2.1(b) demonstrates the result of simulating such a geometric random variable 100 times.

The binomial distribution results if we fix a number of trials at $n \geq 1$, say, and

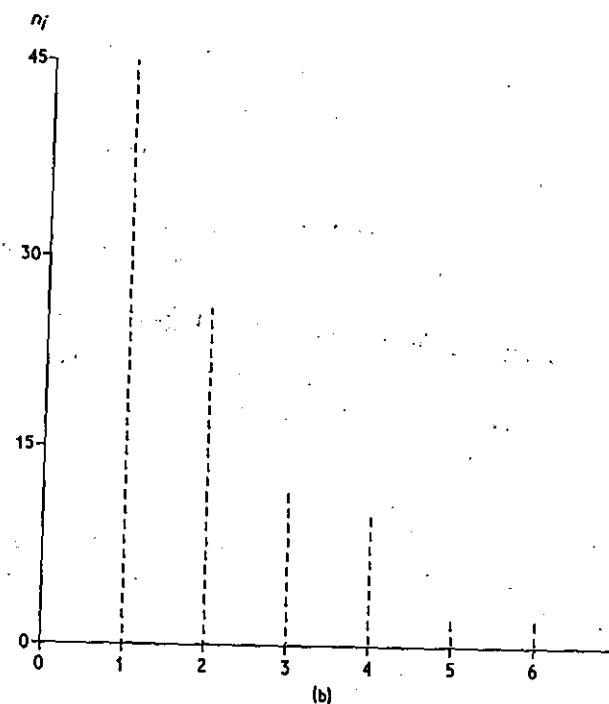
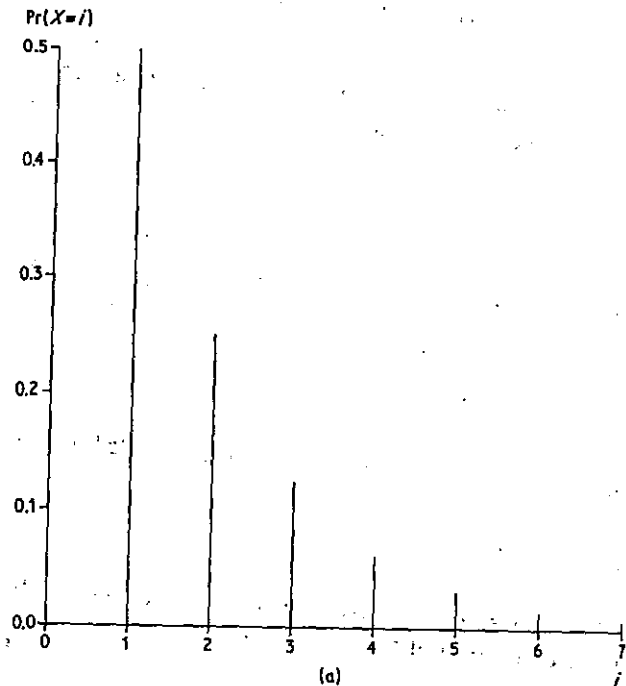
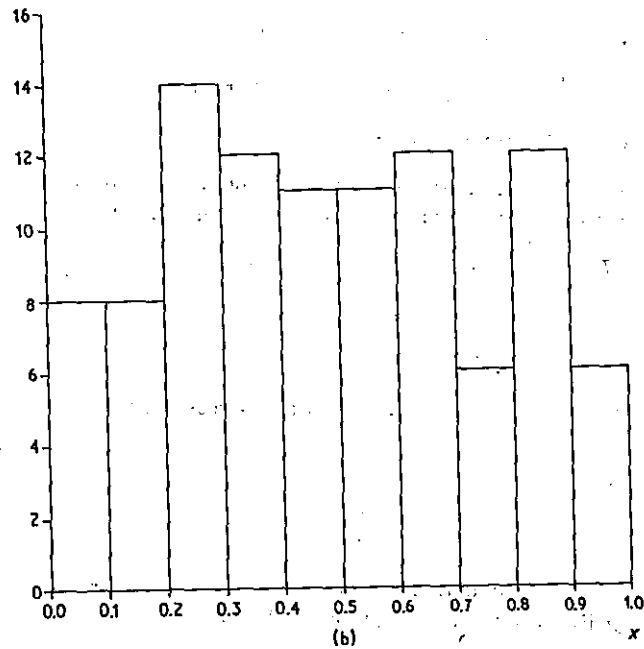
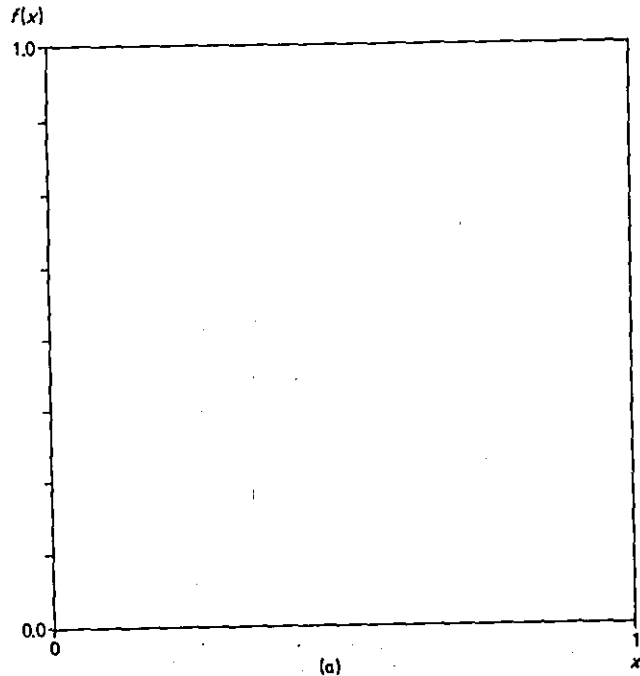


Figure 2.1 (a) Bar-chart illustrating the geometric distribution with $p = 0.5$; (b) Bar-chart illustrating the results from simulating a random variable with the distribution of (a) 100 times. Here i is observed n_i times, $i \geq 1$.

a result which is much used in later chapters. For a $U(0, 1)$ random variable X , $E[X] = \frac{1}{2}$; $\text{Var}(X) = 1/12$. Figure 2.4 illustrates the ' $U(0, 1)$ ' probability density function, and also a histogram resulting from a random sample of size 100 from this density.



2.9 The normal distribution and a central limit theorem

A continuous random variable with a normal distribution, and mean μ and variance σ^2 has the p.d.f.

Normal probability density function:

$$f(x) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] \text{ for } -\infty \leq x \leq \infty$$

Early work on this distribution was by such pioneers as De Moivre, Laplace and Gauss, towards the end of the 18th century and at the start of the 19th century. The normal distribution is so called because of its common occurrence in nature, which is due to 'central limit theorems', which state that, under appropriate conditions, when one adds a large number of random variables, which may well not be normal, the resulting sum has an approximately normal distribution. A formal statement of the commonest central limit theorem is that:

if X_1, X_2, \dots, X_n are independent, identically distributed random variables, with $E[X_i] = \mu$ and $\text{Var}(X_i) = \sigma^2$, then for any real x ,

$$\lim_{n \rightarrow \infty} \Pr\left\{\frac{1}{\sqrt{n}} \sum_{i=1}^n \left(\frac{X_i - \mu}{\sigma}\right) \leq x\right\} = \Phi(x)$$

where $\Phi(x)$ is the c.d.f. of a normal random variable with zero mean and unit variance.

For a more general central limit theorem, and historical background, see Grimmett and Stirzaker (1982, p. 110).

We shall use the notation $N(\mu, \sigma^2)$, to denote the distribution of a normal random variable with mean μ and variance σ^2 . The $N(0, 1)$ case is frequently called the *standard normal*, when the p.d.f. is denoted by $\phi(x)$. Figure 2.5 illustrates $\phi(x)$ and also presents a histogram resulting from a random sample of size 100 from this density.

Figure 2.4 (a) The $U(0, 1)$ probability density function. (b) Histogram summarizing a random sample of size 100 from the density function of (a).

2.10 Exponential, gamma, chi-square and Laplace distributions

We say that a continuous random variable X has an *exponential* distribution with parameter λ when we can write the p.d.f. as

Exponential probability density function:
 $f(x) = \lambda e^{-\lambda x}$ for $0 \leq x < \infty$

$E[X] = 1/\lambda$ and $\text{Var}(X) = 1/\lambda^2$

Some authors (see for example Barnett, 1965) call this the 'negative exponential' p.d.f.

The Poisson process, mentioned in Section 2.7, is often used to model the occurrence of events in time. It predicts that

$\Pr(k \text{ events in a time interval of length } t) = \frac{e^{-\lambda t} (\lambda t)^k}{k!}$ for $0 \leq k < \infty$

where $\lambda > 0$ is the *rate* parameter for the model, and is equal to the average number of events per unit time.

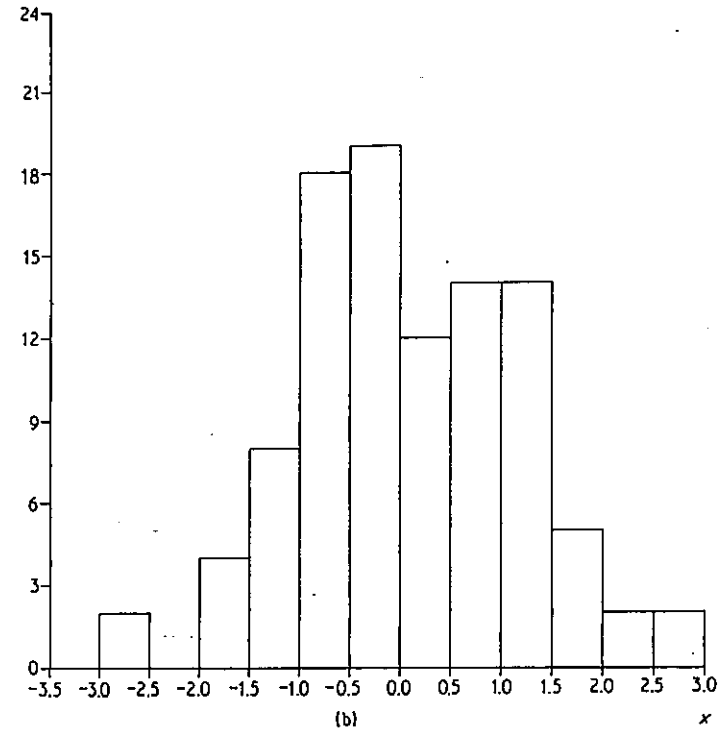
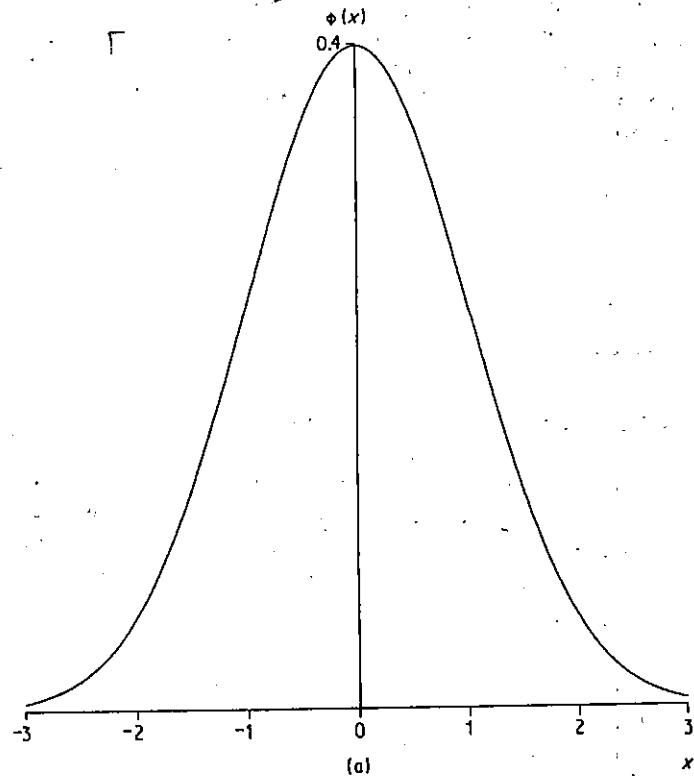


Figure 2.5 (a) The standard normal probability density function,

$\phi(x) = \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-x^2}{2}\right)$ over the range $-3 \leq x \leq 3$. (b) Histogram summarizing a random sample of size 100 from the density function of (a).

If T is a random variable denoting the time to the next event in the Poisson process, measuring time from some arbitrary time origin, then

$\Pr(T \geq t) = \Pr(\text{no events in the time interval } (0, t)) = e^{-\lambda t}$

i.e. $f(t) = \lambda e^{-\lambda t}$

and so times between events in a Poisson process have an exponential distribution.

If we form the sum

$S = \sum_{i=1}^n X_i$

in which the X_i are independent random variables, each with the above exponential distribution, then (see Exercise 2.6 and Example 2.6) S has a

count the number, X , of successes. This gives

Binomial distribution:

$$\Pr(X = i) = \binom{n}{i} p^i q^{n-i} \quad \text{for } 0 \leq i \leq n$$

$$\mathcal{E}[X] = np \quad \text{and} \quad \text{Var}(X) = npq$$

Figure 2.2(a) gives a bar-chart illustrating the binomial distribution for the case $p = 0.5$ and $n = 5$. Figure 2.2(b) demonstrates the result of simulating such a binomial random variable 100 times. We shall refer to such a random variable as possessing a $B(n, p)$ distribution, thus specifying the two parameters, n and p .

A geometric random variable provides the *waiting-time* measured by the number of trials until the first success. The random variable X which measures the waiting-time until the n th success has a *negative-binomial* distribution. When $X = n + i$, for $i \geq 0$, then the $(n + i)$ th trial results in success, and the remaining $(n - 1)$ successes occur during the first $(n + i - 1)$ trials, and we can write

Negative-binomial distribution:

$$\Pr(X = n + i) = \binom{n+i-1}{i} p^i q^n \quad \text{for } 0 \leq i \leq \infty$$

$$\mathcal{E}[X] = n/p \quad \text{and} \quad \text{Var}(X) = nq/p^2.$$

As is shown in Exercise 2.18, there is a simple relationship between the binomial and the negative-binomial distributions.

2.7 The Poisson distribution

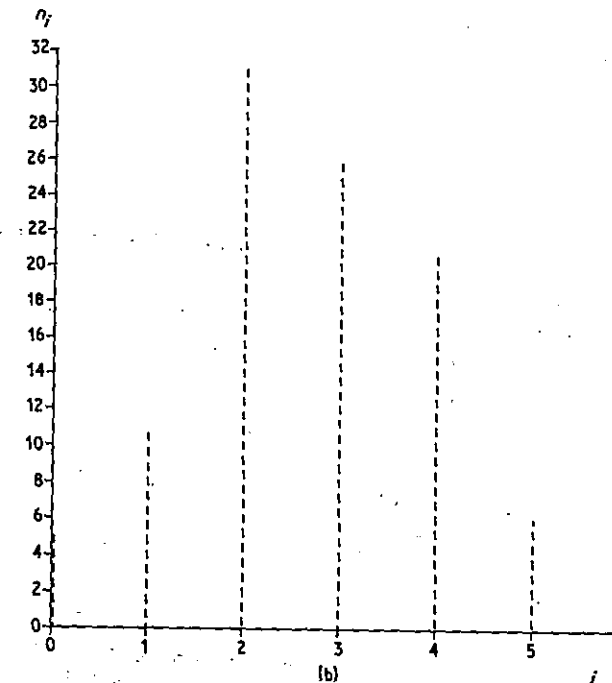
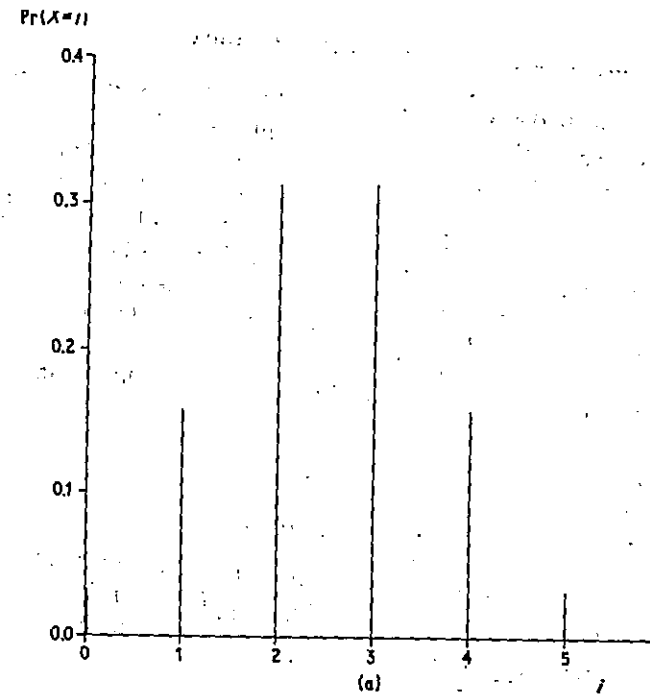
A random variable X with a *Poisson* distribution of parameter λ is described as follows:

Poisson distribution:

$$\Pr(X = i) = \frac{e^{-\lambda} \lambda^i}{i!} \quad \text{for } 0 \leq i \leq \infty$$

$$\mathcal{E}[X] = \lambda \quad \text{and} \quad \text{Var}(X) = \lambda$$

Figure 2.2 (a) Bar-chart illustrating the binomial distribution for the case $n = 5$, $p = 0.5$. (b) Bar-chart illustrating the results from simulating a random variable with the distribution of (a) 100 times. Here i is observed n_i times, $0 \leq i \leq 5$.



Named after the French mathematician, S. D. Poisson, who derived the distribution in 1837, the distribution had been obtained earlier by De Moivre. The Poisson distribution is often useful as a description of data that result when counts are made of the occurrence of events, such as the occurrence of telephone calls in fixed intervals of time, or the numbers of plants within areas of a fixed size. This is because the real-life processes giving rise to the data approximate to a model called a *Poisson process*, which predicts a Poisson distribution for the data. We shall discuss the Poisson process in detail in Section 4.4.2.

Figure 2.3(a) gives a bar-chart illustrating the Poisson distribution for $\lambda = 5$, and Fig. 2.3(b) describes the results of simulating such a Poisson random variable 100 times.

2.8 The uniform distribution

The simplest continuous random variables have uniform (sometimes called rectangular) distributions. As we shall see later, uniform random variables form the basis of most simulation investigations. A uniform random variable over the range $[a, b]$ has the p.d.f.

Uniform p.d.f. over $[a, b]$:

$$f(x) = \frac{1}{(b-a)} \quad \text{for } a < x < b$$

$$f(x) = 0 \quad \text{for } x < a \text{ and } x > b$$

We shall frequently refer to this as the $U(a, b)$ p.d.f., the most important case being when $a = 0$ and $b = 1$.

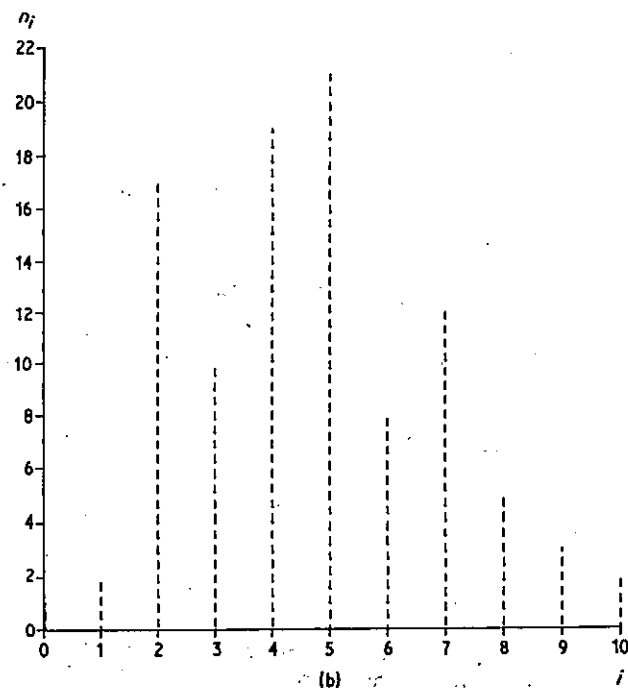
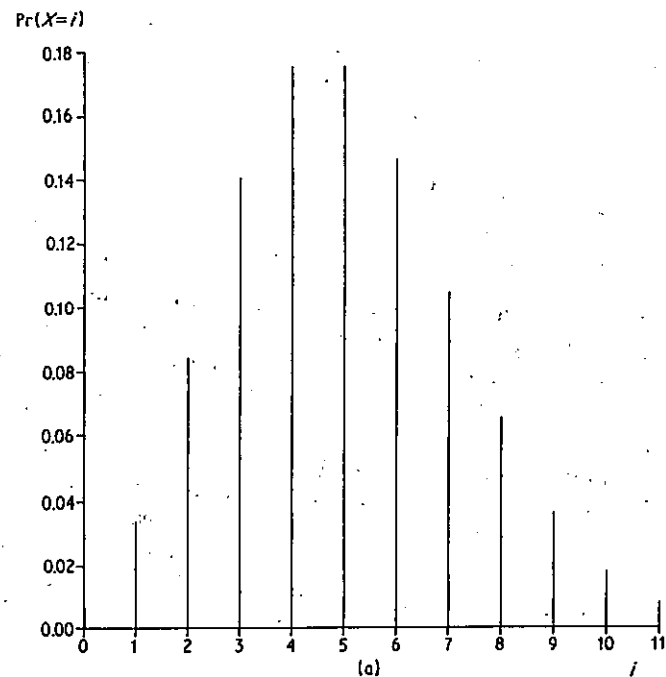
The c.d.f. of a $U(0, 1)$ random variable X is given by

$$F(u) = \int_0^u 1 \, dx = u \quad \text{for } 0 \leq u \leq 1$$

and so for any $0 \leq \alpha \leq \beta \leq 1$,

$$\begin{aligned} \Pr(\alpha \leq X \leq \beta) &= \Pr(0 \leq X \leq \beta) - \Pr(0 \leq X \leq \alpha) \\ &= F(\beta) - F(\alpha) = (\beta - \alpha) \end{aligned}$$

Figure 2.3 (a) Bar-chart illustrating the Poisson distribution for $\lambda = 5$. (b) Bar-chart illustrating the results from simulating a random variable with the distribution of (a) 100 times. Here i is observed n_i times, for $i \geq 0$.



Gamma distribution with the p.d.f.

Gamma probability density function:

$$f(x) = \frac{e^{-\lambda x} \lambda^n x^{n-1}}{\Gamma(n)} \quad \text{for } 0 \leq x < \infty$$

$$\mathcal{E}[X] = n/\lambda \quad \text{and} \quad \text{Var}(X) = n/\lambda^2$$

We shall refer to such a gamma distribution by means of the notation $\Gamma(n, \lambda)$. In this derivation, n is a positive integer, but in general gamma random variables have the above p.d.f. in which the only restriction on n is $n > 0$.

Figure 2.6 presents an exponential p.d.f., and two gamma p.d.f.'s, and a histogram summarizing a random sample of size 100 from the exponential p.d.f.

A random variable with a $\Gamma(v/2, \frac{1}{2})$ distribution is said to have a *chi-square* distribution with parameter v . For reasons which we shall not discuss here, the parameter v is usually referred to as the 'degrees-of-freedom' of the distribution. A random variable X with a $\Gamma(v/2, \frac{1}{2})$ distribution is also said to have a χ^2 distribution, with the p.d.f.

Chi-square probability density function with v degrees of freedom:

$$f(x) = \frac{e^{-x/2} x^{v/2-1}}{\Gamma(v/2) 2^{v/2}} \quad \text{for } x \geq 0$$

$$\mathcal{E}[X] = v \quad \text{and} \quad \text{Var}(X) = 2v$$

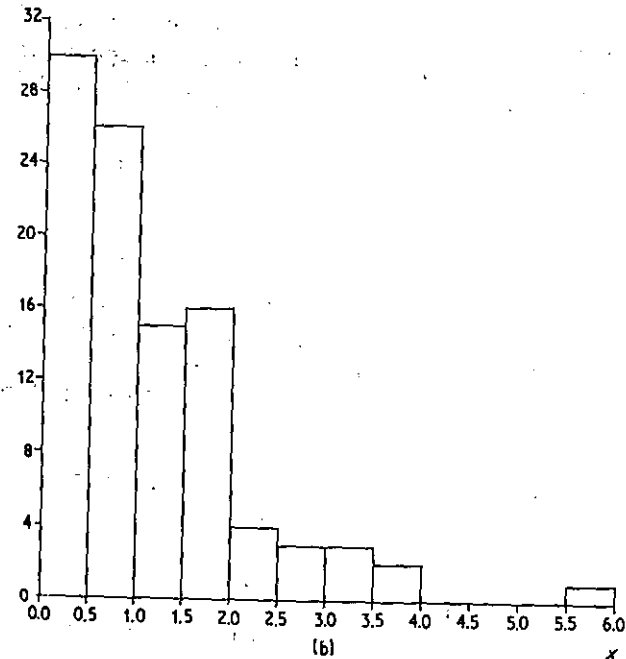
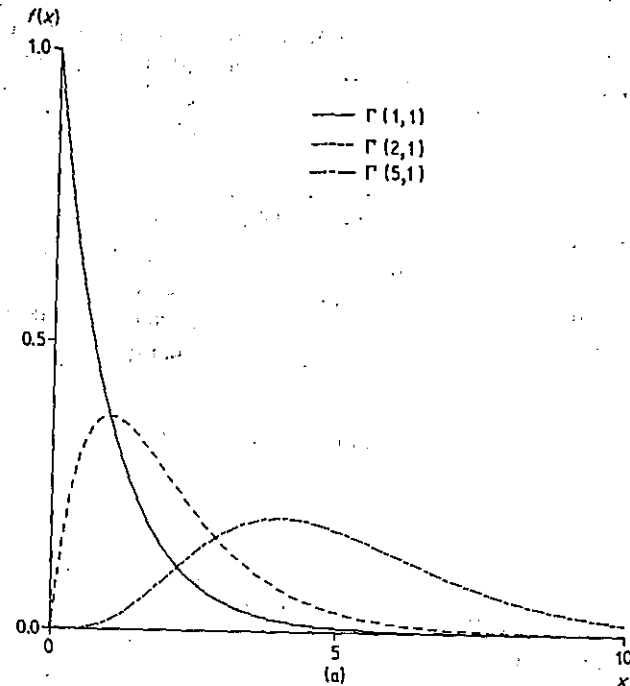
The exponential and gamma distributions describe only non-negative random variables, but the exponential distribution forms the basis of the *Laplace* distribution, discovered by Laplace in 1774 and given below:

Laplace probability density function:

$$f(x) = \frac{\lambda}{2} e^{-\lambda|x|} \quad \text{for } -\infty \leq x \leq \infty$$

$$\mathcal{E}[X] = 0 \quad \text{and} \quad \text{Var}(X) = 2/\lambda^2$$

Figure 2.6 (a) The $\Gamma(1, 1)$ (i.e.; exponential), $\Gamma(2, 1)$ and $\Gamma(5, 1)$ probability density functions. (b) Histogram summarizing a random sample of size 100 from the exponential density function of (a).



Just as the geometric and negative-binomial distributions describe waiting times when time is measured in integer units, the exponential and gamma distributions describe waiting times (in a Poisson process) when time is a continuous quantity, and we shall return to this point again later.

2.11 Distributions of other continuous random variables

Here we shall simply list the standard forms of the p.d.f. of a number of other common continuous random variables to which we shall refer later.

A probability density function that has the same qualitative shape as the normal p.d.f. is the logistic p.d.f., given in standard form below:

The standard logistic probability density function:

$$f(x) = \frac{e^{-x}}{(1 + e^{-x})^2} \quad \text{for } -\infty \leq x \leq \infty$$

$$\mathcal{E}[X] = 0 \quad \text{and} \quad \text{Var}(X) = \pi^2/3$$

We shall later make use of the logistic c.d.f., which in standard form is

$$F(x) = (1 + e^{-x})^{-1} \quad \text{for } -\infty \leq x \leq \infty$$

A unimodal symmetric p.d.f. with more weight in the tails than either the normal or logistic is the Cauchy p.d.f., so called because of its appearance in a paper by Cauchy in 1853. In its standard form the Cauchy p.d.f. is as follows:

The standard Cauchy probability density function:

$$f(x) = \frac{1}{\pi(1 + x^2)} \quad \text{for } -\infty \leq x \leq \infty$$

Because of the large weight in the tails of this p.d.f., a random variable with this distribution does not possess a finite mean or variance.

Finally, we give below the p.d.f. of a random variable with a beta distribution over $[0, 1]$.

The beta probability density function over $[0, 1]$:

$$f(x) = \begin{cases} \frac{x^{\alpha-1} (1-x)^{\beta-1} \Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} & \text{for } 0 < x < 1 \\ 0 & \text{for } x < 0 \text{ and for } x > 1 \end{cases}$$

$$\mathcal{E}[X] = \alpha/(\alpha + \beta) \quad \text{and} \quad \text{Var}(X) = \frac{\alpha\beta}{(\alpha + \beta)^2 (\alpha + \beta + 1)}$$

The beta distribution contains the uniform distribution as a special case: $\alpha = \beta = 1$. If the random variable X has this distribution, then such a beta random variable will be said to have a $B_\alpha(\alpha, \beta)$ distribution.

Figures 2.7–2.9 provide examples of these p.d.f.'s together with histograms summarizing random samples of size 100 from the respective p.d.f.'s

The logistic and Cauchy p.d.f.'s are given in standard, parameter-free form, but we can simply introduce location and scale parameters β and α respectively by means of the transformation $Y = \alpha X + \beta$. This is an example of transforming one random variable to give a new random variable, and we shall now consider such transformations in a general setting.

2.12 New random variables for old

Transforming random variables is a common statistical practice, and one which is often utilized in simulation. The simplest transformation is the linear transformation, $Y = \alpha X + \beta$. In the case of certain random variables, such as uniform, logistic, normal and Cauchy, this transformation does not change the distributional form, and merely changes the distribution parameters, while in other cases the effect of this transformation is a little more complicated.

In the case of single random variables, a general transformation is $Y = g(X)$, for some function g . In such a case, if X is a discrete random variable then the distribution of Y may be obtained by simple enumeration, using the distribution of X and the form of g . Thus, for example, if $Y = X^2$, $\Pr(Y = i) = \Pr(X = -\sqrt{i}) + \Pr(X = \sqrt{i})$. Such enumeration is greatly simplified if g is a strictly monotonic function, so that in the last example, if X were a non-negative random variable then we simply have

$$\Pr(Y = i) = \Pr(X = \sqrt{i})$$

The simplification of the case when g is a strictly monotonic function applies also to the case of the continuous random variables X . Two possible examples are shown in Fig. 2.10.

For the case (a) illustrated in Fig. 2.10, the events $\{Y \leq y\}$ and $\{X \leq x\}$ are clearly equivalent, while for case (b) it is the events $\{Y \geq y\}$ and $\{X \leq x\}$ that are equivalent, so that

$$\left. \begin{array}{l} \text{for case (a), } F(y) = \Pr(Y \leq y) = \Pr(X \leq x) = F(x) \\ \text{and for case (b), } 1 - F(y) = \Pr(Y \geq y) = \Pr(X \leq x) = F(x) \end{array} \right\} \quad (2.1)$$

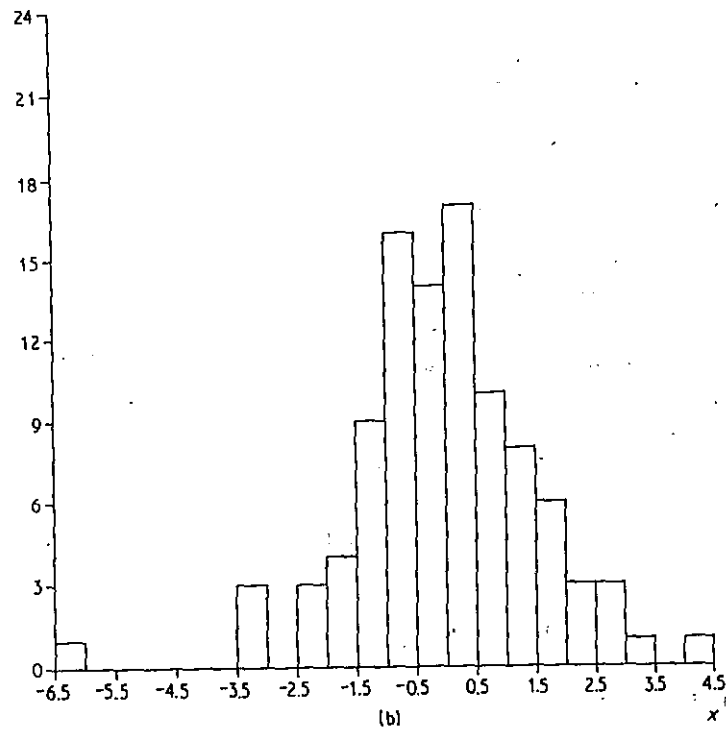
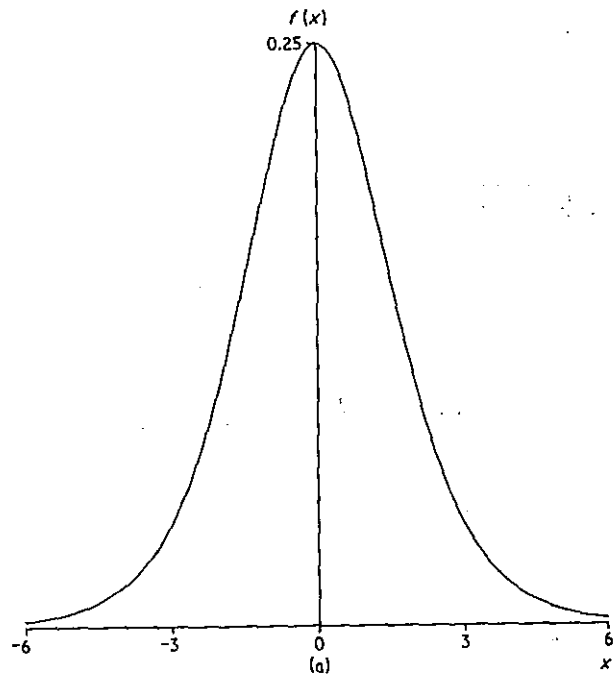


Figure 2.7 (a) The standard logistic density function for $|x| \leq 6$. (b) Histogram summarizing a random sample of size 100 from the density function of (a).

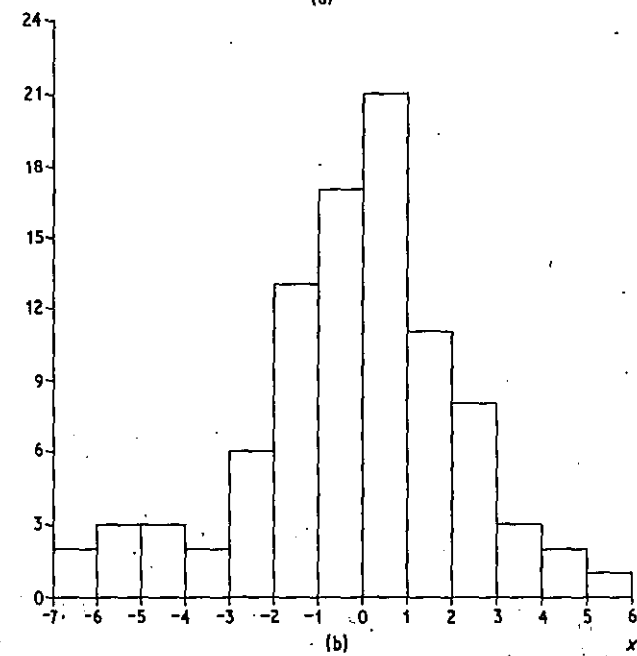
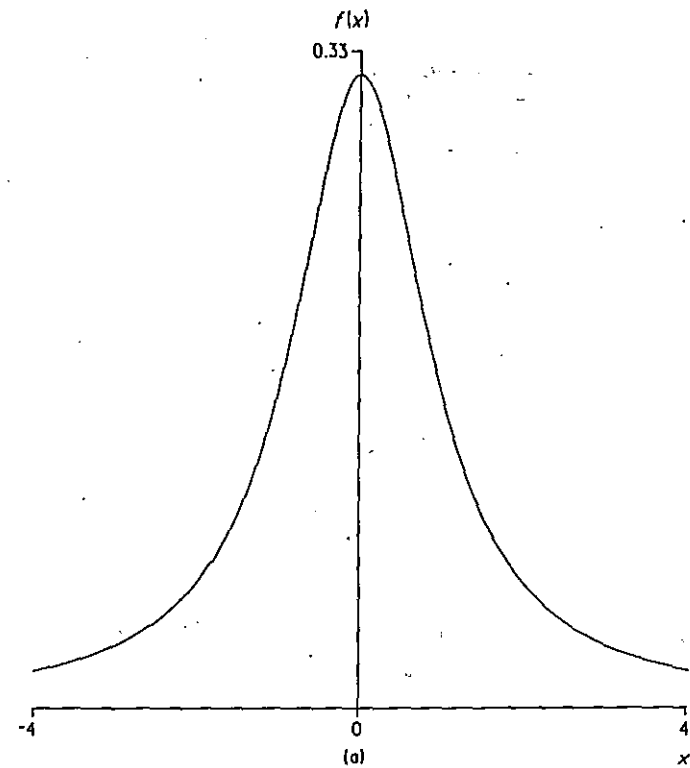


Figure 2.8 (a) The standard Cauchy density function for $|x| \leq 4$. (b) Histogram summarizing a random sample of size 100 from the density function of (a).

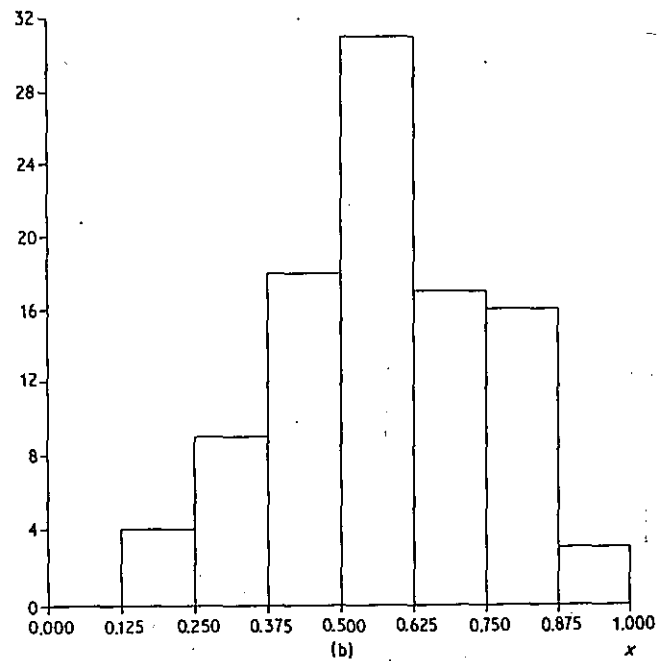
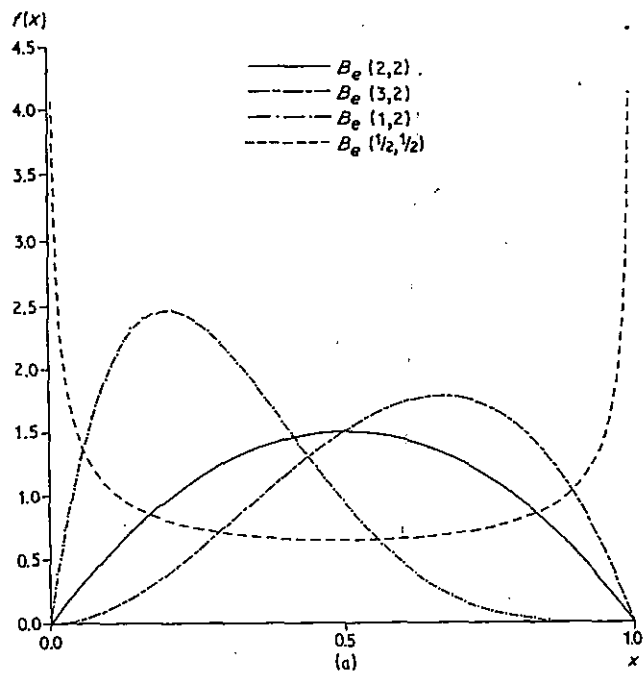


Figure 2.9 (a) The $B_e(2,2)$, $B_e(3,2)$, $B_e(1,2)$ and $B_e(\frac{1}{2}, \frac{1}{2})$ density functions. (b) Histogram summarizing a random sample of size 100 from the $B_e(3,2)$ density function.

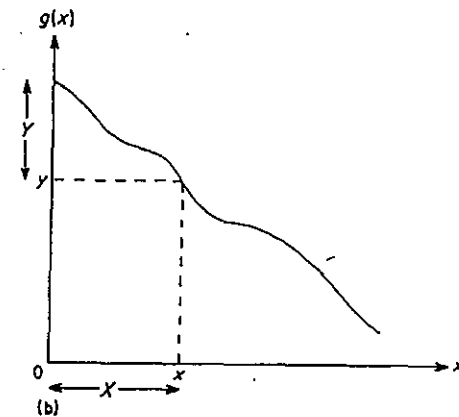
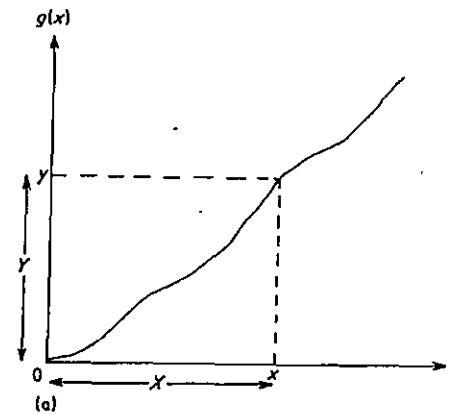


Figure 2.10 Illustrations of $y = g(x)$ where g is strictly monotonic, (a) increasing and (b) decreasing.

leading naturally to:

$$\left. \begin{aligned} f(y) &= f(x) \frac{dx}{dy} && \text{for case (a)} \\ f(y) &= -f(x) \frac{dx}{dy} && \text{for case (b)} \end{aligned} \right\} \quad (2.2)$$

Two examples of case (a) now follow.

EXAMPLE 2.2

$$y = x^2$$

$$f_X(x) = \lambda e^{-\lambda x} \quad \text{for } x \geq 0$$

$$f_Y(y) = \frac{\lambda e^{-\lambda x}}{2x} = \frac{\lambda e^{-\lambda \sqrt{y}}}{2\sqrt{y}}$$

See Fig. 2.11 for the case $\lambda = 1$.

EXAMPLE 2.3

$$y = \sqrt{x}$$

$$f_X(x) = \lambda e^{-\lambda x} \quad \text{for } x \geq 0$$

$$f_Y(y) = 2\lambda y e^{-\lambda y^2}$$

See Fig. 2.12 for the case $\lambda = 1$.

We can see from Figs 2.11 and 2.12 how the two different transformations have put different emphases over the range of x , resulting in the two different forms for $f_Y(y)$ shown. Thus in Fig. 2.12, 'small' values of x are transformed into larger values of y (for $0 < x < 1$, $\sqrt{x} > x$), with the result that the mode of $f_Y(y)$ is to be found at $y = \sqrt{1/2\lambda} > 0$. However, in Fig. 2.11, for $0 < x < 1$, $x^2 < x$, and the mode of $f_Y(y)$ remains at 0.

The aim in the above has been to obtain $f(y)$ as a function of y alone, and to do this we have substituted $x = g^{-1}(y)$. Cases (a) and (b) in Equation (2.2) are both described by:

$$f_Y(y) = f_X(g^{-1}(y)) \left| \frac{dx}{dy} \right| \quad (2.3)$$

If g does not have a continuous derivative, then strictly (2.3) does not hold without a clear specification of what is meant by dx/dy . In practice, however, such cases are easily dealt with when they arise (see Exercise 2.25), since the appropriate result of Equation (2.1) always holds, giving $F(y)$.

The result of (2.3) is very useful in the simulation of random variables, as we shall see later. It may be generalized to the case of more than one random variable, when the derivative of (2.3) becomes a Jacobian. Thus, for example, if

$$w = g(x, y)$$

and

$$z = h(x, y)$$

provide us with a one-to-one transformation from (x, y) to (w, z) , then the Jacobian of the transformation is given by the determinant

$$J = \begin{vmatrix} \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} \\ \frac{\partial z}{\partial x} & \frac{\partial z}{\partial y} \end{vmatrix}$$

and if $J \neq 0$ and all the partial derivatives involved are continuous, we can write the joint density of W and Z as:

$$f_{W,Z}(w, z) = f_{X,Y}(x, y) |J^{-1}| \quad (2.4)$$

As with the case of a single random variable, we express the right-hand side of (2.4) as a function of w and z only. It is sometimes useful to note that

$$J^{-1} = \begin{vmatrix} \frac{\partial x}{\partial w} & \frac{\partial x}{\partial z} \\ \frac{\partial y}{\partial w} & \frac{\partial y}{\partial z} \end{vmatrix}$$

It often occurs that we require the distribution of the random variable, $W = g(X, Y)$. Introduction of some suitable function, $Z = h(X, Y)$, may result in a one-to-one transformation, so that (2.4) will give the joint density function of W and Z , from which we may then derive the required density of W as the marginal density:

$$f_W(w) = \int f_{W,Z}(w, z) dz$$

(See Exercises 2.14 and 2.15 for examples.) We shall now consider an example of the use of (2.4).

EXAMPLE 2.4

Let N_1 and N_2 be independent $N(0, 1)$ normal random variables. The pair (N_1, N_2) defines a point in two dimensions, by Cartesian co-ordinates. The transformation, from Cartesian to polar co-ordinates given by

$$N_1 = R \cos \Theta$$

$$N_2 = R \sin \Theta$$

is one-to-one, and all the partial derivatives involved are continuous, so that we

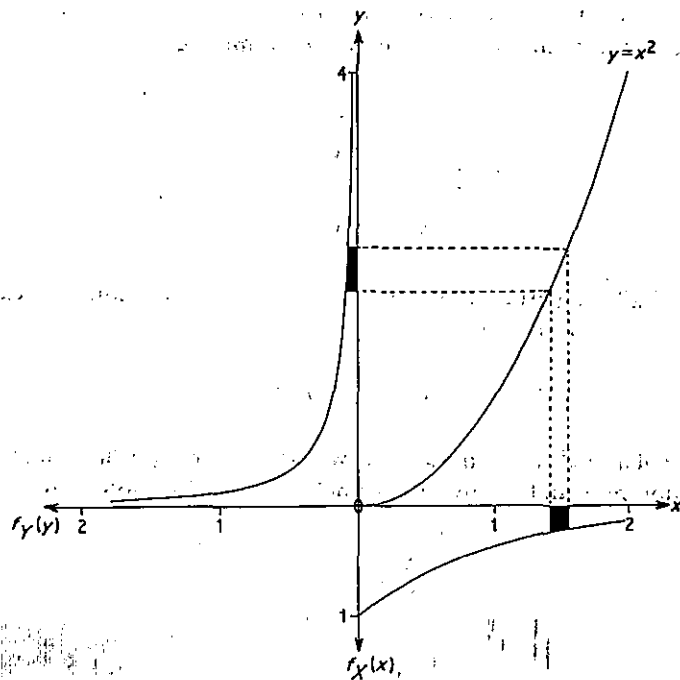


Figure 2.11. An illustration of the transformation $y = x^2$ and the densities $f_X(x) = e^{-x}$, $f_Y(y) = \frac{e^{-\sqrt{y}}}{2\sqrt{y}}$. The shaded regions have the same area.

may use (2.4) to derive the joint density function R and Θ as follows:

$$J^{-1} = \begin{vmatrix} \frac{\partial n_1}{\partial r} & \frac{\partial n_1}{\partial \theta} \\ \frac{\partial n_2}{\partial r} & \frac{\partial n_2}{\partial \theta} \end{vmatrix} = \begin{vmatrix} \cos \theta & -r \sin \theta \\ \sin \theta & r \cos \theta \end{vmatrix} = r$$

$$\begin{aligned} \text{Thus } f_{R\Theta}(r, \theta) &= \frac{r}{2\pi} \exp\left[-\frac{1}{2}(n_1^2 + n_2^2)\right] \\ &= \frac{r}{2\pi} \exp\left[-r^2/2\right] \quad \text{for } 0 \leq \theta \leq 2\pi, 0 \leq r \leq \infty. \end{aligned}$$

We thus see that R and Θ are independent random variables, with $f_\Theta(\theta) = 1/2\pi$, i.e. Θ is uniform over $[0, 2\pi]$, and $f_R(r) = r \exp[-r^2/2]$, i.e. (see Example 2.3), R^2 has an exponential distribution of parameter $\frac{1}{2}$.

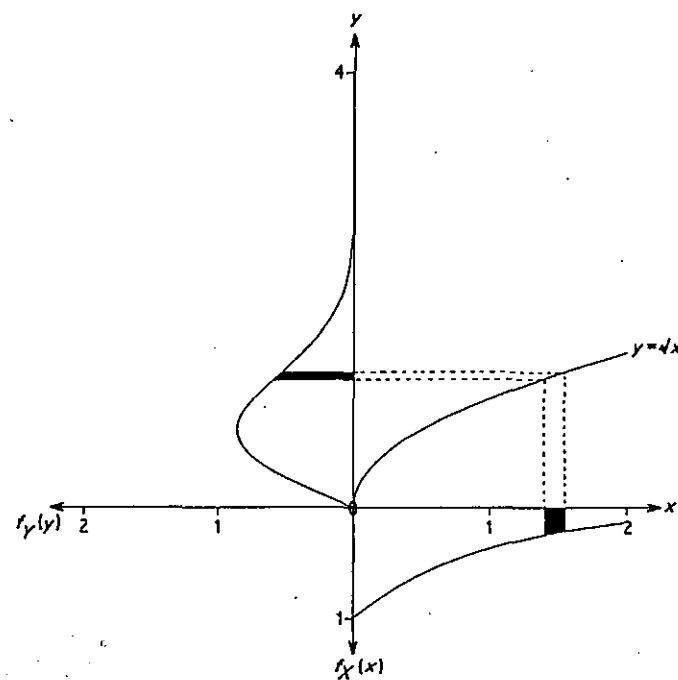


Figure 2.12. An illustration of the transformation $y = \sqrt{x}$ and the densities $f_X(x) = e^{-x}$, $f_Y(y) = 2ye^{-y^2}$. The shaded regions have the same area.

2.13 Convolutions

We have seen earlier that a further common transformation is a linear combination of a number of independent random variables. Again, in some cases the distributional form of the components of the sum is preserved, as occurs with Poisson, normal and Cauchy random variables, for example, while in other cases the distributional form changes, as when a sum of independent exponential random variables has a gamma distribution, as we have seen above.

The sum of mutually independent random variables is called a *convolution*. Its distribution may be evaluated by a convolution sum, or integral, as appropriate, as can be seen from the two examples that now follow.

EXAMPLE 2.5

Suppose X_1 has a $B(n_1, p)$ distribution, X_2 has a $B(n_2, p)$ distribution, and that X_1 and X_2 are independent.

Let $S = X_1 + X_2$

$$\begin{aligned} \Pr(S = k) &= \sum_{i=0}^{\min(k, n_1)} \Pr(X_1 = i) \Pr(X_2 = k - i) \\ &= \sum_{i=0}^{\min(k, n_1)} \binom{n_1}{i} p^i (1-p)^{n_1-i} \binom{n_2}{k-i} p^{k-i} (1-p)^{n_2-k+i} \\ &= p^k (1-p)^{n_1+n_2-k} \sum_{i=0}^{\min(k, n_1)} \binom{n_1}{i} \binom{n_2}{k-i} \end{aligned}$$

which can be shown to equal:

$$\binom{n_1+n_2}{k} p^k (1-p)^{n_1+n_2-k} \quad \text{for } 0 \leq k \leq n_1+n_2$$

Thus S has a $B(n_1+n_2, p)$ distribution.

EXAMPLE 2.6

Suppose X_1 and X_2 are independent exponential random variables, each with the p.d.f. $\lambda e^{-\lambda x}$ for $x \geq 0$.

Let $S = X_1 + X_2$

$$\begin{aligned} f_S(s) &= \int f_{X_1}(x) f_{X_2}(s-x) dx \\ &= \int_0^s \lambda^2 e^{-\lambda x} e^{-\lambda(s-x)} dx \\ &= \lambda^2 e^{-\lambda s} \quad \text{for } s \geq 0 \end{aligned}$$

i.e. S has a $\Gamma(2, \lambda)$ distribution.

The result of this last example was anticipated in Section 2.10, and further examples of convolutions are given in Exercises 2.5–2.8. An important and often difficult feature in the evaluation of convolution sums and integrals is the correct determination of the admissible range for the convolution sum or integral.

2.14 The chi-square goodness-of-fit test

In the above figures illustrating distributions we can see the good qualitative match between the shapes of distributions and the corresponding shapes of histograms or bar-charts. For larger samples we would expect this match to

improve. Whatever the sample size, however, we can ask whether the match between, say, probability density function and histogram is good enough. This is an important question when it comes to testing a procedure for simulating random variables of a specific type.

Special tests exist for special distributions, and we shall encounter some of these in Chapter 6; however, a test, due to K. Pearson, exists which may be applied in any situation. When this test was established by Pearson in 1900 it formed one of the cornerstones of modern statistics. The test refers to a situation in which, effectively, balls are being placed independently in one of m boxes. For any distribution we can divide up the range of the random variable into m disjoint intervals, observe how many of the simulated values (which now correspond to the balls) fall into each of the intervals (the boxes), and compare the observed numbers of values in each interval with the numbers we would expect. We then compute the statistic,

$$X^2 = \sum_{i=1}^m \frac{(O_i - E_i)^2}{E_i}$$

where we have used O_i and E_i to denote respectively the observed and expected numbers of values in the i th interval. If the random variables are indeed from the desired distribution then the X^2 statistic has, asymptotically, a chi-square distribution on an appropriate number of degrees of freedom. The rule for computing the degrees of freedom is

$$\text{degrees of freedom} = \text{number of intervals} - 1 - \text{number of parameters, suitably estimated, if any}$$

This test is useful because of its universal applicability, but simply because it may be applied in general it tends not to be very powerful at detecting departures from what one expects. A further problem with this test is that the chi-square result only holds for 'large' expected values. Although in many cases this may simply mean that we should ensure $E_i > 5$, for all i , we may well have to make a judicious choice of intervals for this to be the case. For further discussion, see Everitt (1977, p. 40), and Fienberg (1980, p. 172). The distribution of X^2 when cell values are small is discussed by Fienberg; this case may be investigated by simulation, and an illustration is given in Section 9.4.1. We shall use this test in Chapter 6 (see also Exercise 2.24).

*2.15 Multivariate distributions

In the last section we encountered the simplest of all multivariate distributions, the multinomial distribution, which results when we throw n balls independently into m boxes, with $p_i = \Pr(\text{ball lands in the } i\text{th box})$, for $1 \leq i \leq m$ and $\sum_{i=1}^m p_i = 1$.

Here we have a family of random variables, $\{X_i, 1 \leq i \leq m\}$, where X_i denotes the number of balls falling into the i th box; and so $\sum_{i=1}^m X_i = n$. The joint distribution of these random variables is given below:

Multinomial distribution:

$$\Pr(X_i = x_i, 1 \leq i \leq m) = \binom{n}{x_1, x_2, \dots, x_m} \prod_{i=1}^m p_i^{x_i},$$

where $\sum_{i=1}^m x_i = n$ and $\sum_{i=1}^m p_i = 1$

Here

$$\binom{n}{x_1, x_2, \dots, x_m} = \frac{n!}{x_1! x_2! \dots x_m!},$$

the multinomial coefficient.

An important continuous multivariate distribution is the multivariate normal distribution, also called the multi-normal distribution. In its bivariate form the multivariate normal density function is

Bivariate normal probability density function:

$$\phi(x_1, x_2) = \frac{1}{2\pi\sigma_1\sigma_2(1-\rho^2)^{1/2}} \exp \left\{ -\frac{1}{2(1-\rho^2)} \left[\left(\frac{x_1 - \mu_1}{\sigma_1} \right)^2 - 2\rho \left(\frac{x_1 - \mu_1}{\sigma_1} \right) \left(\frac{x_2 - \mu_2}{\sigma_2} \right) + \left(\frac{x_2 - \mu_2}{\sigma_2} \right)^2 \right] \right\}$$

for $-\infty < x_1, x_2 < \infty$

Here ρ is the correlation between the two random variables; Fig. 2.13 illustrates two possible forms for $\phi(x_1, x_2)$. The p -variate density function has the following form:

p -variate multivariate normal probability density function:

$$\phi(\mathbf{x}) = (2\pi)^{-p/2} |\Sigma|^{-1/2} \exp \left(-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})' \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right)$$

for $-\infty < x_i < \infty, 1 \leq i \leq p$

notation used: $N(\boldsymbol{\mu}, \Sigma)$

Here $\boldsymbol{\mu}$ is the mean vector, $(\mathbf{x} - \boldsymbol{\mu})'$ is the transpose (row vector) of the column

vector $(\mathbf{x} - \boldsymbol{\mu})$, and Σ is the variance/covariance matrix, i.e. $\Sigma = \{\sigma_{ij}, 1 \leq i, j \leq p\}$, in which σ_{ij} is the covariance between the component random variables X_i and X_j . Thus σ_{ii} is the variance of X_i , for $1 \leq i \leq p$.

It can readily be shown (see, e.g., Morrison, 1976, p. 90, and cf. Exercise 2.16) that if $\mathbf{Y} = \mathbf{A}\mathbf{X}$ and \mathbf{X} has the $N(\boldsymbol{\mu}, \Sigma)$ distribution, where \mathbf{A} is a nonsingular $p \times p$ matrix, then \mathbf{Y} has the $N(\mathbf{A}\boldsymbol{\mu}, \mathbf{A}\Sigma\mathbf{A}')$ distribution.

*2.16 Generating functions

The material of this section is not used extensively in the remainder of the book, and many readers may prefer to move on to Section 2.17.

It is often convenient to know the forms of *generating functions* of random variables. For any random variable X , we define the moment generating function (m.g.f.) as

$$M_X(\theta) = \mathcal{E}[e^{\theta X}]$$

for an appropriate range of the dummy variable, θ . Not all random variables have m.g.f.'s: the Cauchy distribution provides a well-known example. However, if $M_X(\theta)$ exists for a nontrivial interval for θ , then the m.g.f.

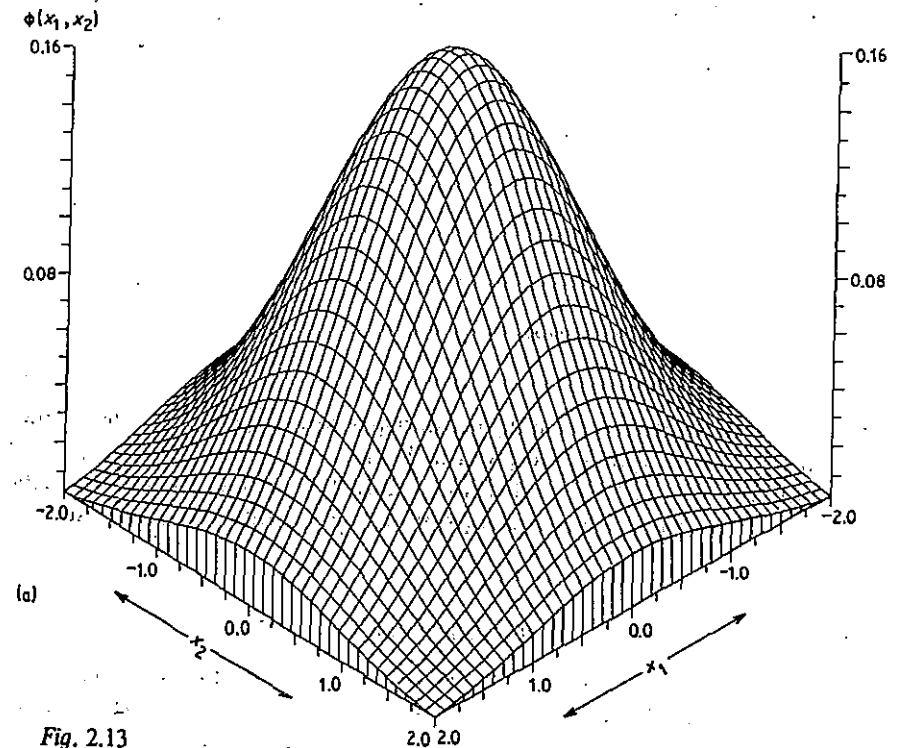


Fig. 2.13

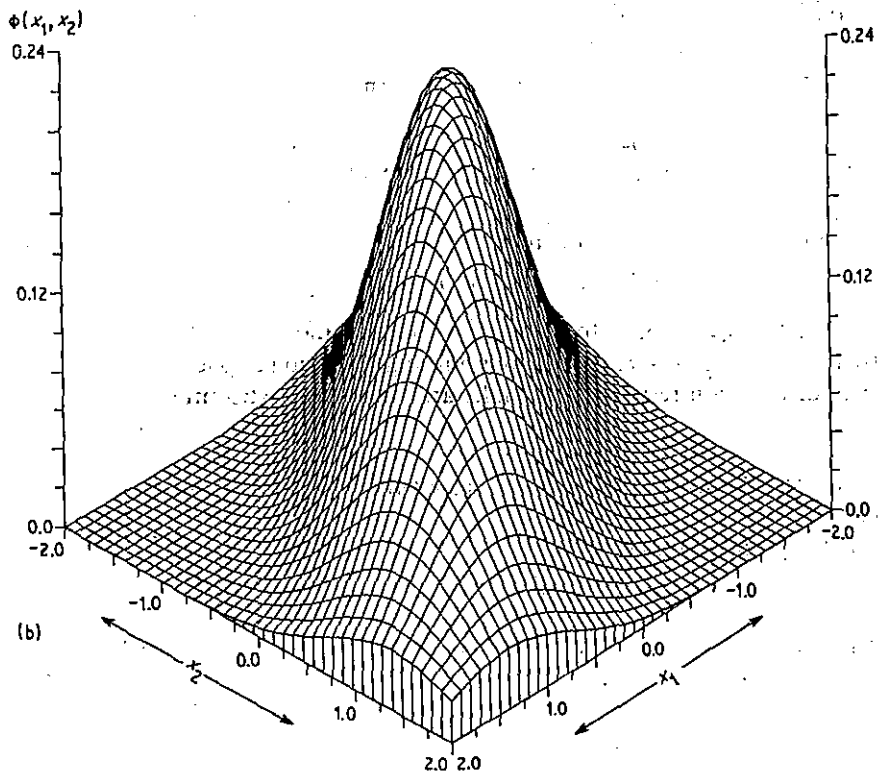


Figure 2.13 Illustration of the bivariate normal density function for the cases

- (a) $\mu_1 = \mu_2 = 0, \sigma_1 = \sigma_2 = 1, \rho = 0$
- (b) $\mu_1 = \mu_2 = 0, \sigma_1 = \sigma_2 = 1, \rho = 0.5$

characterizes the random variable. An alternative generating function is the probability generating function, defined by

$$G(z) = \mathcal{E}[z^X]$$

M.g.f.'s for some of the distributions considered earlier in this chapter are given in Table 2.1.

For the distributions of Table 2.1, the m.g.f. may be used to check the values of means and variances given earlier, since

$$M'(0) = \mathcal{E}[X], \text{ and } M''(0) = \mathcal{E}[X^2],$$

illustrating why the m.g.f. is so named.

A glance at the m.g.f.'s of Table 2.1 shows that binomial, negative-binomial and gamma random variables can be expressed as convolutions of identically

Table 2.1 Common distributions and associated moment generating functions

Distribution	m.g.f.
geometric: $\Pr(X = i) = q^{i-1}p$	$pe^\theta(1 - qe^\theta)^{-1}$, for $qe^\theta < 1$
binomial: $B(n, p)$: $\Pr(X = i) = \binom{n}{i} p^i q^{n-i}$	$(q + pe^\theta)^n$
negative-binomial: $\Pr(X = n + i) = \binom{n+i-1}{i} p^i q^n$	$p^n e^{n\theta} (1 - qe^\theta)^{-n}$, for $qe^\theta < 1$
Poisson: $\Pr(X = i) = \frac{e^{-\lambda} \lambda^i}{i!}$	$e^{\lambda(e^\theta - 1)}$
normal: $N(0, 1)$: $f(x) = \frac{e^{-x^2/2}}{\sqrt{2\pi}}$	$e^{\theta^2/2}$
exponential: $f(x) = \lambda e^{-\lambda x}$	$\frac{\lambda}{\lambda - \theta}$ for $\theta < \lambda$
gamma: $\Gamma(n, \lambda)$: $f(x) = \frac{e^{-\lambda x} \lambda^n x^{n-1}}{\Gamma(n)}$	$\left(\frac{\lambda}{\lambda - \theta}\right)^n$ for $\theta < \lambda$

distributed random variables. We see why this is so as follows:

Let
$$S = \sum_{i=1}^n X_i$$

then
$$M_S(\theta) = \mathcal{E}\left[\exp\left(\theta \sum_{i=1}^n X_i\right)\right]$$

$$= \mathcal{E}\left[\prod_{i=1}^n \exp(\theta X_i)\right]$$

and if the $\{X_i\}$ are mutually independent, then

$$M_S(\theta) = \prod_{i=1}^n \mathcal{E}[\exp(\theta X_i)] = \prod_{i=1}^n M_{X_i}(\theta).$$

Furthermore, if the $\{X_i\}$ have the common m.g.f., $M_X(\theta)$, say, then

$$M_S(\theta) = (M_X(\theta))^n \tag{2.5}$$

Thus, for example, a random variable X with the $\Gamma(n, \lambda)$ distribution can be written as

$$X = \sum_{i=1}^n E_i$$

where the E_i are independent, identically distributed exponential random variables with parameter λ (cf. Exercise 2.6).

Moment generating functions may also be defined for m jointly distributed random variables X_1, X_2, \dots, X_m , as follows:

$$M_X(\theta) = \mathcal{E} \left[\prod_{i=1}^m \exp(\theta_i X_i) \right]$$

Thus for the multinomial distribution of Section 2.15, we have the multivariate moment generating function

$$M_X(\theta) = \left(\sum_{i=1}^m p_i \exp \theta_i \right)^n$$

while the multivariate normal distribution of Section 2.15 has the multivariate m.g.f.

$$M_X(\theta) = \exp(\theta' \mu + \frac{1}{2} \theta' \Sigma \theta)$$

A bivariate Poisson distribution which we shall encounter later is simply defined by its m.g.f.:

$$M_X(\theta) = \exp[\lambda_1 (e^{\theta_1} - 1) + \lambda_2 (e^{\theta_2} - 1) + \lambda_3 (e^{\theta_1 + \theta_2} - 1)] \quad (2.6)$$

We shall conclude this section with two examples which complement work earlier in the chapter and illustrate further the utility of generating functions.

EXAMPLE 2.7 Proof of a central limit theorem

A $B(n, p)$ random variable W can be written as a convolution:

$$W = \sum_{i=1}^n X_i$$

where $\mathcal{E}[X_i] = p$ and $\text{Var}(X_i) = pq$, where $q = 1 - p$.

$$\text{Let } S_n = \frac{(W - np)}{\sqrt{(npq)}}$$

$$\begin{aligned} \text{then } M_{S_n}(\theta) &= \mathcal{E} \left[\exp \left(\frac{(W - np)\theta}{\sqrt{(npq)}} \right) \right] \\ &= \mathcal{E} \left[\exp \left(\sum_{i=1}^n (X_i - p)\phi \right) \right] \end{aligned}$$

where $\phi = \theta / \sqrt{(npq)}$

and so by (2.5), as the $\{X_i\}$ are independent,

$$M_{S_n}(\theta) = (M_Y(\phi))^n, \quad \text{where } Y = (X_i - p)$$

From the above, $\mathcal{E}[Y] = 0$ and $\mathcal{E}[Y^2] = pq$, and so

$$\begin{aligned} M_{S_n}(\theta) &= \left(1 + \frac{\phi^2 pq}{2} + \text{higher order terms in } \phi \right)^n \\ &= \left(1 + \frac{\theta^2}{2n} + \text{higher order terms in } \left(\frac{\theta}{\sqrt{n}} \right) \right)^n \end{aligned}$$

and by a result similar to that of Exercise 2.22,

$$M_{S_n}(\theta) \rightarrow \exp(\theta^2/2) \text{ as } n \rightarrow \infty.$$

Thus as $n \rightarrow \infty$ the m.g.f. of $S_n \rightarrow$ the m.g.f. of an $N(0, 1)$ random variable, and so the distribution of $S_n \rightarrow N(0, 1)$. A similar limiting operation applied to the multinomial distribution results in the multivariate normal distribution.

EXAMPLE 2.8 Deriving the Poisson distribution from the binomial distribution

If W has a $B(n, p)$ distribution, then

$$M_W(\theta) = (1 - p + pe^\theta)^n$$

Now let us keep $np = \lambda$, say, fixed, while we let $n \rightarrow \infty$ (and consequently $p \rightarrow 0$).

$$\text{Now } M_W(\theta) = \left(1 + \frac{\lambda(e^\theta - 1)}{n} \right)^n,$$

and as $n \rightarrow \infty$, $M_W(\theta) \rightarrow \exp[\lambda(e^\theta - 1)]$, (see Exercise 2.22)

i.e. the m.g.f. of a Poisson random variable with parameter λ . Hence under this limiting operation the distribution of W tends to this Poisson form.

It is possible to derive the exponential and gamma distributions by similar limiting processes applied, respectively, to the geometric and negative-binomial distributions (see Exercise 2.23). This approach may be used to provide an heuristic proof that the rules of the Poisson process result in a predicted Poisson distribution (see Parzen, 1960, p. 253).

2.17 Discussion and further reading

While we have dichotomized random variables as usually discrete or continuous, we have not mentioned, for instance, that most discrete random variables simply take integer values. Furthermore, the continuous random variables we have considered are, formally, absolutely continuous random

variables. Such discussion is not necessary for the material to follow, but it may be found in books such as Blake (1979) and Parzen (1960). Additional discrete and continuous distributions will arise throughout the book.

In this chapter we have presented only the tip of a very large iceberg. Much more detail can be found in, for example, Haight (1967), Johnson and Kotz (1969, 1970a, 1970b and 1972), Kendall and Stuart (1961) and Ord (1972). Mardia (1970) considers families of bivariate distributions, while Douglas (1980) describes the interesting distributions which can result from special combinations of distributions such as the binomial and Poisson. Cramér (1954) discusses and proves different forms of central limit theorems, and Bailey (1964), Cox and Miller (1965) and Feller (1957) provide the necessary background to the Poisson process. Apostol (1963) is a good reference for the full transformation-of-variable theory, which is also well described by Blake (1979). Further discussion of the chi-square goodness-of-fit test is provided by Cochran (1952) and Craddock and Flood (1970), whose small-sample study is the subject of Section 9.4.1. A more leisurely introduction to some of the material of this chapter is provided by Folks (1981), and Cox and Smith (1967) provide a good introduction to the mathematical theory of queues, relevant to Exercises 2.26–2.28.

2.18 Exercises and complements

(a) Transforming random variables

- 2.1 Derive the density function of the random variable

$$X = -\log_e U, \text{ where } U \text{ is } U(0, 1).$$

- 2.2 Consider the effect of the transformation $Y = aX$, where a is a fixed constant, and X is, e.g., an exponential, normal, gamma, or Poisson random variable.

- 2.3 Show that if X has the distribution of Exercise 2.1, and $W = \gamma X^{1/\beta}$ then W has a Weibull distribution with p.d.f.

$$f_W(\omega) = \frac{\beta}{\gamma^\beta} \omega^{\beta-1} \exp[-(\omega/\gamma)^\beta]$$

for $0 \leq \omega < \infty$, $\beta > 0$, $\gamma > 0$.

- 2.4 Find the distribution of $Y = N^2$, where N is an $N(0, 1)$ random variable.

- 2.5 If Y_1, Y_2, \dots, Y_n are all mutually independent $N(0, 1)$ random variables, show, by induction or otherwise, that $\sum_{i=1}^n Y_i^2$ has the χ_n^2 distribution.

- 2.6 If Y_1, Y_2, \dots, Y_n are all mutually independent exponential random

variables with p.d.f. $\lambda e^{-\lambda y}$ for $\lambda > 0$, $y \geq 0$, show, by induction, and using the convolution integral, that $\sum_{i=1}^n Y_i$ has the $\Gamma(n, \lambda)$ distribution.

- *2.7 If Y_1, Y_2, \dots, Y_n are all mutually independent Cauchy random variables with p.d.f. $(\pi(1+y^2))^{-1}$, derive the distribution of $1/n \sum_{i=1}^n Y_i$.

- 2.8 X, Y are independent random variables. Find the distribution of $X+Y$ when:

- (a) X, Y are $N(\mu_1, \sigma_1^2), N(\mu_2, \sigma_2^2)$ respectively.
 (b) X, Y are Poisson, with parameters λ, μ , respectively
 (c) X, Y are exponential, with parameters λ, μ , respectively.

- 2.9 If X, Y are as in Exercise 2.8(b), find

$$\Pr(X = r | X+Y = n) \quad 0 \leq r \leq n.$$

- 2.10 If X and Y are independent random variables, find the distribution of $Z = \max(X, Y)$ in terms of the c.d.f.'s of X and Y .

- *2.11 X_1, X_2, \dots, X_n are independent random variables with the distribution of Exercise 2.1. Prove that the following random variables have the same distribution:

$$Y = \max(X_1, X_2, \dots, X_n)$$

$$Z = X_1 + \frac{X_2}{2} + \dots + \frac{X_n}{n}.$$

- *2.12 Random variables Y_1 and Y_2 have the exponential p.d.f. e^{-x} for $x \geq 0$. Let $X_1 = Y_1 - Y_2$ and $X_2 = Y_1 + Y_2$. Find the joint distribution of (X_1, X_2) .

- *2.13 Let X_1, X_2 be two independent and identically distributed non-negative continuous random variables. Find the joint probability density function of $\min(X_1, X_2)$ and $|X_1 - X_2|$. Deduce that these two new random variables are independent if and only if X_1 and X_2 have an exponential distribution. In such a case, evaluate $\Pr(X_1 + X_2 \leq 3 \min(X_1, X_2) \leq 3b)$, where b is constant.

- 2.14 Random variables X, Y are independently distributed as χ_{2a}^2 and χ_{2b}^2 respectively. Show that the new random variables, $S = X+Y$ and $T = X/(X+Y)$ are independent, and T has a beta, $B_e(a, b)$ distribution.

- *2.15 If N_1, N_2, N_3, N_4 are independent $N(0, 1)$ random variables, show that:

- (a) $X = |N_1 N_2 + N_3 N_4|$ has the exponential p.d.f. e^{-x} for $x \geq 0$.
 (b) $C = N_1/N_2$ has the Cauchy distribution of Exercise 2.7.

- *2.16 X is a p -dimensional column vector with the multivariate $N(0, I)$

distribution, in which $\mathbf{0}$ denotes a p -variate zero vector and \mathbf{I} is the $p \times p$ identity matrix. If $\mathbf{Z} = \mathbf{A}\mathbf{X} + \boldsymbol{\mu}$, where \mathbf{A} is an arbitrary $p \times p$ matrix, and $\boldsymbol{\mu}$ is an arbitrary p -dimensional column vector, show that \mathbf{Z} has the $N(\boldsymbol{\mu}, \mathbf{A}\mathbf{A}')$ distribution.

(b) Manipulation of random variables, and questions arising from the chapter

- *2.17 Two independent Poisson processes have parameters λ_1 and λ_2 . Find and identify the distribution of the number of events in the first process which occur before the first event in the second process.
- *2.18 Random variables X and Y have the related distributions:

$$\Pr(Y = k) = \binom{n+m}{k} (1-\theta)^k \theta^{n+m-k} \quad \text{for } 0 \leq k \leq n+m$$

$$\Pr(X = k) = \binom{n+k-1}{k} \theta^k (1-\theta)^n \quad \text{for } k \geq 0$$

Here n, m are positive integers, and $0 < \theta < 1$, so that Y is binomial, and X is negative-binomial. By finding the coefficient of z^i in $(1+z)^{n+m}/(1+z)^{m+1-i}$, for $0 \leq i \leq m$, or otherwise, show that

$$\Pr(X \leq m) = \Pr(Y \geq n).$$

- *2.19 Use a central limit theorem approach to show that

$$\lim_{n \rightarrow \infty} e^{-n} \sum_{r=0}^n \frac{n^r}{r!} = \frac{1}{2}.$$

- *2.20 Show that a random variable with the negative-binomial distribution has the moment generating function

$$M_X(\theta) = p^n e^{n\theta} (1 - qe^\theta)^{-n}.$$

- *2.21 Show that a random variable with the gamma $\Gamma(n, \lambda)$ distribution has the moment generating function

$$\left(\frac{\lambda}{\lambda - \theta} \right)^n \quad \text{for } \theta < \lambda.$$

- *2.22 Show that $\lim_{n \rightarrow \infty} \left(1 + \frac{x}{n} \right)^n = e^x$.

- *2.23 Suppose X is a random variable with a geometric distribution of parameter p . Let $Y = aX$. If $a \rightarrow 0$ and $p \rightarrow 0$ in such a way that $\lambda = a/p$ is a constant, show that the distribution of Y tends to that of a random variable with an exponential distribution with parameter λ^{-1} .

- 2.24 Use the chi-square goodness-of-fit test to compare the observed and expected values in the intervals: (0, 0.1), (0.1, 0.2), etc., for the example of Fig. 2.4, arising from the $U(0, 1)$ distribution. The grouped data frequencies are, in increasing order: 8, 8, 14, 12, 11, 11, 12, 6, 12, 6.
- 2.25 X is a random variable with the exponential p.d.f., e^{-x} for $x \geq 0$. We define Y as follows:

$$\begin{aligned} \text{for } 0 \leq X \leq 1, & \quad Y = X \\ \text{for } X \geq 1, & \quad Y = 2X - 1. \end{aligned}$$

Obtain the distribution of Y .

(c) Questions on modelling, continuing Exercises 1.4, 1.6 and 1.7

- 2.26 The simple queue of Exercise 1.4 measured time in integral units. More realistically, times between arrivals, and service times, would be continuous quantities, sometimes modelled by random variables with exponential distributions. Observe a real-life queue, at a post-office, for example, make a record of inter-arrival and service times and illustrate these by means of histograms. What underlying distributions might seem appropriate?

- 2.27 (continuation) The BASIC program given below simulates what is called an M/M/1 queue (see e.g., Gross and Harris, 1974, p. 8). In this queue, inter-arrival times are independent random variables with $\lambda e^{-\lambda x}$ exponential density function, and service times are independent random variables with $\mu e^{-\mu x}$ exponential density function. There is just one server and $\lambda/(\lambda + \mu)$ plays the rôle of p in Exercise 1.4. Run this program for cases: $\lambda = \mu$, $\lambda > \mu$ and $\lambda < \mu$, and comment on the results.

NOTE that the statements 100, 150 and 190 below simulate a $U(0, 1)$ random variable. The method used by the computer is described in the next chapter. The function of statements 110 and 160 should be clear from the solutions to Exercises 2.1 and 2.2. An explanation of why this program does in fact simulate an M/M/1 queue is given in Section 8.3.1.

```

10 REM THIS PROGRAM SIMULATES AN M/M/1 QUEUE, STARTING EMPTY
20 REM AS INPUT YOU MUST PROVIDE ARRIVAL AND DEPARTURE RATES
30 REM NOTE THAT THERE IS NO TERMINATION RULE IN THIS PROGRAM
40 PRINT "TYPE LAMBDA AND MU, IN THAT ORDER"
50 INPUT L,M
60 LET S=L+M
70 LET I=L/S
80 PRINT "QUEUE SIZE.....AFTER TIME"
90 RANDOMIZE
100 LET U=RND
110 LET E=(-LOG(U))/L
120 REM E IS THE TIME TO FIRST ARRIVAL AT AN EMPTY QUEUE

```

```

130 LET Q = 1
140 PRINT Q,E
150 LET U = RND
160 LET E = (-LOG(U))/S
170 REM E IS TIME TO NEXT EVENT, IE., ARRIVAL OR DEPARTURE
180 REM WE MUST NOW FIND THE TYPE OF THAT EVENT
190 LET U = RND
200 IF U > I THEN 250
210 REM THUS WE HAVE AN ARRIVAL
220 LET Q = Q+1
230 PRINT Q,E
240 GOTO 150
250 REM THUS WE HAVE A DEPARTURE
260 LET Q = Q-1
270 PRINT Q,E
280 IF Q = 0 THEN 100
290 GOTO 150
300 END
    
```

*2.28 (continuation) We have seen that exponential distributions result from Poisson processes, and we can consider the parameters λ and μ of Exercise 2.27 to be rate parameters in Poisson processes for arrivals and departures, respectively. In some cases it may seem realistic for λ and μ each to be functions of the current queue size, n , say. For example, if $\lambda_n = 2/(n+1)$ and $\mu = 1$, we have simple 'discouragement' queue, with an arrival rate which decreases with increasing queue size. Modify the BASIC program of Exercise 2.27 in order to simulate this discouragement queue, and compare the behaviour of this queue with that of the M/M/1 queue with $\lambda = 2$, $\mu = 3$. We shall continue discussion of these queues in Chapters 7 and 8.

3

GENERATING UNIFORM RANDOM VARIABLES

3.1 Uses of uniform random numbers

Random digits are used widely in statistics, for example, in the generation of random samples (see Barnett, 1974, p. 22), or in the allocation of treatments in statistical experiments (see Cox, 1958, p. 72). More generally still, uniform random numbers and digits are needed for the conduct of lotteries, such as the national premium bond lottery of the United Kingdom (see Thompson, 1959).

A further use for random digits is given in the following example.

EXAMPLE 3.1

The randomized response technique

In conducting surveys of individuals' activities it may be of interest to ask a question which could be embarrassing to the interviewee; possible examples include questions relating to car driving offences, sex, tax-evasion and the use of drugs. Let us denote the embarrassing question by E , and suppose, for the population in question, we know the frequency, p , of positive response to some other, non-embarrassing, question, N , say. We can now proceed by presenting the interviewee with both questions N and E , and a random digit simulator, producing 0 with probability p_0 , and producing 1 with probability $1 - p_0$. The interviewee is then instructed to answer N if the random digit is 0, say, and to answer E if the random digit is 1. The interviewer does not see the random digit. From elementary probability theory (see ABC, p. 85)

$$\begin{aligned} \Pr(\text{response} = \text{Yes}) &= \Pr(\text{response} = \text{Yes} | \text{question is } N)p_0 \\ &+ \Pr(\text{response} = \text{Yes} | \text{question is } E)(1 - p_0) \end{aligned}$$

Knowing p_0 and $\Pr(\text{response} = \text{Yes} | \text{question is } N)$, and estimating $\Pr(\text{response} = \text{Yes})$ from the survey, enables one to estimate $\Pr(\text{response} = \text{Yes} | \text{question is } E)$. This illustration is an example of a randomized-

response technique (RRT), and for further examples and discussion, see Campbell and Joiner (1973) and Exercises 3.1–3.4.

Uniform random numbers are clearly generally useful. Furthermore, in Chapters 4 and 5 we shall see that if we have a supply of $U(0, 1)$ random variables, we can simulate any random variable, discrete or continuous, by suitably manipulating these $U(0, 1)$ random variables.

Initially, therefore, we must consider how we can simulate uniform random variables, the *building-blocks* of simulation, and that is the subject of this chapter. We start by indicating the relationships between discrete and continuous uniform random variables.

3.2 Continuous and discrete uniform random variables

If U is a $U(0, 1)$ random variable, and we introduce a discrete random variable D such that

$$D = i \text{ if and only if } i \leq 10U < i+1, \quad \text{for } i = 0, 1, 2, \dots, 9$$

then $\Pr(D = i) = \Pr(i \leq 10U < i+1)$

$$= \frac{1}{10} \quad \text{for } i = 0, 1, 2, \dots, 9$$

The random variable D thus provides equi-probable (uniform) random digits.

Conversely, if we write a $U(0, 1)$ random variable, U , in decimal form,

$$U = \sum_{k \geq 1} D(k) 10^{-k}$$

Then intuitively we would expect $D(k)$ to be a uniform random digit, for each $k \geq 1$,

$$\text{i.e. } \Pr(D(k) = i) = \frac{1}{10}, \quad \text{for } 0 \leq i \leq 9,$$

$$\text{and } k \geq 1$$

This and further results are proved by Yakowitz (1977, pp. 29–31). We see, therefore, that $U(0, 1)$ random variables can readily give us uniform random digits, while given a means of simulating random digits we can combine them to give $U(0, 1)$ variables to whatever accuracy is required.

3.3 Dice and machines

The simplest random number generators are coins, dice and bags of coloured balls, the very bread-and-butter of exercises in elementary probability theory.

Thus in the RRT example above, the interviewee could be given a well-shaken bag of balls, a proportion p_0 of which are white, with the remainder being black. Without looking, the interviewee then selects a ball from the bag, and answers question N if the ball chosen is white, and answers question E if the ball chosen is black. Similar physical devices are sometimes used in lotteries, and games of chance such as bingo and roulette. Certain countries such as Australia, Canada, France and West Germany televise, once a week, the operation of a complex physical device for selecting winning lottery numbers. West (1955) provides an analysis of the results of a lottery carried out in Rhodesia.

The random digits we usually need are uniform over the 0–9 range, and such digits can be obtained by suitably manipulating simple devices such as coins, as in the following example:

EXAMPLE 3.2

A fair coin is tossed four times. If we record a head as 0 and a tail as 1, then the result of the experiment is four digits, $abcd$, written in order, e.g., 0110. We can interpret $abcd$ as the number, $(a \times 2^3) + (b \times 2^2) + (c \times 2) + d$, so that 0110 is interpreted as 6. If the resulting number is greater than 9, we reject it and start again. If the resulting number is in the 0–9 range then it is a realization of a uniformly distributed random digit over that range. (Based on part of an A-level question, Oxford, 1978.)

We can see this simply by enumerating the possible outcomes to the experiment:

Outcome	Resulting number
0000	0
1000	8
0100	4
0010	2
0001	1
1100	12
1010	10
1001	9
0110	6
0101	5
0011	3
1110	14
1101	13
1011	11
0111	7
1111	15

We are just using the coin to simulate the binary form of the digits 0–15. This method therefore does give rise to uniform random digits over 0–9, but it is rather wasteful, as resulting numbers are rejected 3/8 of the time.

Manipulations of this kind are avoided by the direct use of simple dice to produce 0–9 uniform random digits. Unfortunately, a regular 10-sided figure does not exist, but one can use icosahedral dice (giving regular 20-sided figures), each digit 0–9 appearing separately on two different faces. Further possibilities include rolling a regular 10-faced cylinder, or throwing a 10-faced di-pyramid, with each face being an isosceles triangle of some fixed size. These simple devices are illustrated in Fig. 3.1.



Figure 3.1 (a) Three icosahedral dice. Note the need to distinguish between 6 and 9 (b) A regular, 10-faced cylinder (c) Three 10-faced di-pyramids, with truncated isosceles triangles of the same size as faces. Note that the two pyramids are so attached that when the body is at rest a face is uppermost.

Because of the general demand for random digits, tables, such as those of Appendix 2, are now widely available. A sequence of random digits can be obtained by reading the table by rows, by columns, or by any other rule. The first table of this kind was produced by Tippett in 1927, and it was regarded as a 'godsend' by the statisticians of the day (Daniels, 1982).

In using physical devices such as dice to simulate random digits one is reversing the customary model/reality relationship. As described in Chapter 1, one usually takes a real-life situation, and builds a model of it. Here we start with a model, such as a uniform random digit, seek a real-life mechanism to correspond to that model, and then take observations from the real-life mechanism. There is always a discrepancy between model and reality—coins may not be fair (see, e.g., Kerrich, 1946), dice may be biased, and so on—therefore the numbers produced by physical devices are tested, to ensure that no drastic non-randomness is present. This is simply a form of quality control of random numbers, and one applies only a finite subset of the infinity of tests that are possible. We shall return to the subject of testing of numbers in Chapter 6.

Any process in nature that is thought to be random may be used to try to simulate uniform random numbers. Kendall and Babbington-Smith (1939a) used a rotating disk with ten uniform segments, which was stopped at random. Tippett (1925) used digits read from tables of logarithms. ERNIE, the computer used for selecting winning premium bonds in the British national lottery, uses the electronic 'noise' of neon tubes. The digits of Table 3.1 were obtained from reading the last three digits of successive numbers from the Canterbury region telephone directory. (Cf. Section 6.7 and Exercise 6.8. The relative frequencies of these digits are considered in Example 6.1.)

Student (1908a) drew samples from a set of physical measurements taken on criminals, as described in Section 1.5. In his case we have an illustration of sampling from a non-uniform population, (approximately normal in this case), and similarly exponential and Poisson random variables may be simulated directly if one can observe a process in nature which provides a good approximation to a Poisson process (see Section 4.4.2).

Dice and machines are impractical for all but the smallest simulations, which are now in any case likely to be conducted with the aid of readily available tables (see for instance, Neave, 1981, and Murdoch and Barnes, 1974). Large-scale simulations are usually conducted using computers, and early computers were equipped with built-in random-number generators of the physical kind, using random electronic features, as in ERNIE. Tocher (1975, chapter 5) provides many examples here, and even circuit diagrams. More recently, Isida (1982) presented a compact physical random-number generator based on the noise of a Zener diode. The modern equivalent of this can be found in certain hand-calculators, which have an RND button for simulating $U(0, 1)$ random variables. A problem with all physical devices is the danger that they may

Table 3.1 Digits from telephone numbers

	874	580	873	824	564	663
	478	658	540	561	360	082
	661	839	996	261	052	938
	334	420	356	571	081	866
	569	166	045	091	961	610
(a)	471	378	936	569	107	022
	916	865	961	838	303	826
	665	014	148	764	276	638
	504	776	237	682	634	207
	659	654	774	217	609	684
	423	213	423	002	960	273
	183	059	563	379	252	955
	202	410	451	887	467	427
(b)	207	483	809	265	117	891
	061	658	145	950	135	495
	716	232	955	771	747	699
	693	757	952	053	659	459
	991	876	091	431	316	283
	499	223	743	037	891	729
	611	998	650	527	073	665

become unreliable, through changes to the device in time; thus dice, for instance, could become unevenly worn, resulting in bias. Frequent checks of the generated numbers should therefore be carried out.

The modern approach to large-scale simulation is quite different from that of this section, and it avoids the need for such frequent checking by producing a sequence of numbers that can be shown mathematically to possess certain desirable features. This approach, which is also not without its drawbacks, is described in the next section.

3.4 Pseudo-random numbers

The digits of Table 3.2 superficially have the appearance of the digits of Table 3.1, but they have been generated in a blatantly non-random fashion, from the recursion formula

$$u_{n+1} = \text{fractional part of } (\pi + u_n)^5 \quad \text{for } n \geq 0 \quad (3.1)$$

where u_0 is some specified number in the range $0 < u_0 < 1$. u_0 is, rather graphically, termed the 'seed'. Knowledge of the formula of (3.1) provides one with complete knowledge of the sequence of numbers resulting in Table 3.2., but in many applications one may find these digits as suitable as those, say, of Table 3.1, and much more easily generated on a calculator or computer. Formula (3.1) can be likened to a 'black box' which takes the place of a physical black-box such as a die. Recursion formulae are most suitable for use on computers

Table 3.2 Digits from the recursion of Equation (3.1).

254	032	329	233	252	444
794	807	600	974	884	454
797	354	440	855	159	290
162	053	737	489	953	381
051	091	224	843	075	513
703	740	755	750	070	002
301	810	903	392	970	915
690	642	767	038	140	051
962	283	420	435	835	150
574	108	551	564	209	788
810	657	491	939	365	537
612	514	020	950	567	239
119	865	638	032	062	491
966	619	460	553	850	096
255	550	872	019	601	282
474	943	141	486	022	074
013	589	023	454	681	854
489	857	712	412	307	910
826	305	753	610	885	458
346	008	309	763	890	300

Each triple is obtained from the first three decimal places of the u_n , when (3.1) was operated using a 32-bit computer and floating-point arithmetic. Successive numbers were obtained moving from left to right across the rows, and down the table.

and calculators, and furthermore the properties of the numbers they produce can be investigated mathematically. If the resulting numbers satisfy a variety of tests, then because of the deterministic nature of a recursion formula, additional application of these tests at a later stage is not necessary, as there is no danger of bias creeping into the black box, with the progress of time.

In some applications it may be required to re-run a simulation using the same random numbers as on a previous run. Such a requirement may seem unlikely, but we shall see in Chapter 7 that it can be very useful in certain methods for variance-reduction. Knowledge of u_0 for a formula such as (3.1) enables one to do this quite easily, whereas such a 're-run' facility is not possible with physical generators unless a possibly time-consuming record is made of the numbers used. Inoue *et al.* (1983) describe the generation and testing of random digits which may be supplied on magnetic tapes.

3.5 Congruential pseudo-random number generators

An alternative mathematical representation of formula (3.1) is:

$$u_{n+1} = (\pi + u_n)^5 \pmod{1} \quad \text{for } n \geq 0$$

Currently the recursion formula that is most frequently adopted is:

$$x_{n+1} = ax_n + b \pmod{m} \quad \text{for } n \geq 0 \quad (3.2)$$

in which a , b and m are suitably chosen fixed integer constants, and the seed is an integer, x_0 . Starting from x_0 , the formula (3.2) gives rise to a sequence of integers, each of which lies in the 0 to $(m-1)$ range. Because the resulting numbers can be investigated by the theory of congruences, such generators are termed 'congruential'. Although terminology is not always uniform here, we shall call a generator with $b=0$, 'multiplicative', and one with $b \neq 0$, 'mixed'.

Approximations to $U(0, 1)$ variables can be obtained from setting $u_i = x_i/m$, as discussed in Exercise 3.15. For an example, see the solution to Exercise 3.21.

Formulae such as (3.1) are sometimes used to play games involving random elements on hand calculators. We can examine the numbers produced and we may find that they satisfy many criteria of random numbers. However, there is no guarantee, in general, that at some stage the sequence of numbers produced by such formulae may not seriously violate criteria of random numbers, and thus, in general, such formulae are of little use for scientific work. As we shall see, an advantage of the formula (3.2) is that certain guarantees are available for the resulting numbers.

The constants a , b and m are chosen with a number of aims in mind. For a start, one wants the arithmetic to be efficient. Human beings do arithmetic to base 10, and so if the formula (3.2) was being operated by hand, using pencil and paper, it would be sensible for m to be some positive integral power of 10.

For example, if we have

$$x_0 = 89, a = 1573, b = 19, m = 10^3$$

then from (3.2),

$$\begin{aligned} x_1 &= 140\,016 \pmod{10^3} = 16 \\ x_2 &= 25\,187 \pmod{10^3} = 187 \\ &\text{etc.} \end{aligned}$$

Clearly, if one naturally does arithmetic to number base r , say, then the operation of division by m is most efficiently done if $m = r^k$ for some positive integer k . For most computers this entails setting $m = 2^k$, where k is selected so that m is 'large' (see below) and the numbers involved are within the accuracy of the machine.

A moment's thought shows that the generator of (3.2) can produce no more than m different numbers before the cycle repeats itself again and again. Thus a second aim in choosing the constants a , b , m is that the cycle length, which could certainly be less than m , is reasonably large. It has been shown (see Hull and Dobell, 1962; and Knuth, 1981, pp. 16-18) that for the case $b > 0$, the maximum possible cycle length m is obtained if, and only if, the following relations hold:

- (i) b and m have no common factors other than 1;

- (ii) $(a-1)$ is a multiple of every prime number that divides m ;
 (iii) $(a-1)$ is a multiple of 4 if m is a multiple of 4.

If $m = 2^k$, relation (iii) will imply that $a = 4c + 1$ for positive integral c . Such an a then also satisfies relation (ii). When $m = 2^k$, relation (i) is easily obtained by setting $b = \text{any odd positive constant}$. Proofs of results such as these are usually given in general number-theoretic terms; however, following Peach (1961), in Section 3.9 we provide a simple proof of the above result for the commonly used case: $m = 2^k$, $a = 4c + 1$ and b odd (c , b , and k positive integers).

Although multiplicative congruential generators involve less arithmetic than mixed congruential generators, it is not possible to obtain the full cycle length in the multiplicative case. Nevertheless, if $m = 2^k$ for a multiplicative generator, then a cycle length of 2^{k-2} may be obtained. This is achieved by setting $a \equiv \pm 3 \pmod{8}$, and now also imposing a constraint on x_0 , namely, choosing x_0 to be odd. A suitable choice for a is an odd power of 5, since, for positive, integral q ,

$$\begin{aligned} 5^{2q+1} &= (1+4)^{2q+1} = (1+4(2q+1)) \pmod{8} \\ &= -3 \pmod{8} \end{aligned}$$

Five such generators that have been considered are:

a	k
5^{13}	36, 39
5^{17}	40, 42, 43

For further discussion of multiplicative congruential generators, see Exercise 3.31.

When one first encounters the idea of a sequence of 'random' numbers cycling, this is disturbing. However, it is put in perspective by Wichmann and Hill (1982a), who present a generator, which we shall discuss later, with a cycle length greater than 2.78×10^{13} . As they remark, if one used 1000 of these numbers a second, it would take more than 800 years for the sequence to repeat.

Large cycle lengths do not necessarily result in sequences of 'good' pseudo-random numbers, and a third aim in the choice of a , b , m is to try to produce a small correlation between successive numbers in the series; for truly random numbers, successive numbers are uncorrelated, but we can see that this is not likely to be the case for a generator such as (3.2). Greenberger (1961) has shown

that an approximation to the correlation between x_n and x_{n+1} is given by:

$$\rho \approx \frac{1}{a} - \frac{6b}{am} \left(1 - \frac{b}{m}\right) \pm \frac{a}{m} \quad (3.3)$$

Greenberger gives the following two examples of sequences with the same full cycle length:

	a	b	m	ρ
(i)	$2^{34} + 1$	1	2^{35}	0.25
(ii)	$2^{18} + 1$	1	2^{35}	$\ll 2^{-18}$

Expressions such as (3.3) are obtained by averaging over one complete cycle of a full-period mixed generator (cf. Exercise 3.13) and exact formulae for ρ , involving Dedekind sums, are presented by Kennedy and Gentle (1980, p. 140). As is discussed by Kennedy and Gentle, and also by Knuth (1981, p. 84), choosing a , b and m to ensure small ρ can result in a poor generator in other respects. For instance, for sequences that are much shorter than the full cycle, the correlation between x_n and x_{n+1} may be appreciably higher than the value of ρ for the complete cycle. Also, higher-order correlations may be far too high; see Coveyou and MacPherson (1967) and Van Gelder (1967) for further discussion. It is sometimes recommended that one takes $a \approx \sqrt{m}$ (see e.g., Cooke, Craven and Clarke, 1982, p. 69). However, this approximate relationship holds for the RANDU generator, originally used by IBM and, as we can see from Exercise 3.25, this generator possesses a rather glaring Achilles heel. Unfortunately, as we shall see in Chapter 6, this is a defect which can be hard to detect using standard empirical tests. As a further example, $a \approx \sqrt{m}$ for the generator of Exercise 3.31 (ii), which passes the randomness tests of Downham and Roberts (1967) yet has since been shown to have undesirable properties by Atkinson (1980). Similar findings for this generator and that of Exercise 3.31 (i) are given by Grafton (1981).

The choice of the constants a , b and m is clearly a difficult one; but the convenience of pseudo-random number generators has made the search for good generators worth while. Ultimately, the properties of any generator will be judged by the use intended for the numbers to be generated, and by the tests applied. A very important feature of congruential generators, which is perhaps inadequately emphasized, is that the arithmetic involved in operating the formula (3.2) is exact, without any round-off error. Thus naïve programming of the formula (3.2) in, say, BASIC can rapidly result in a sequence of unknown properties, because of the use of floating-point arithmetic; this feature is clearly illustrated in Exercise 3.14. This problem is usually solved in computer implementations by machine-code programs which employ integer arithmetic.

In this case the modulus operation can be performed automatically, without division, if the modulus, $m = 2^r$, and r is the computer word size: after $(ax_{i-1} + b)$ is formed, then only the r lowest-order bits are retained; this is the integer 'overflow or carry-out' feature described by Kennedy and Gentle (1980, p. 19).

3.6 Further properties of congruential generators

One might well expect numbers resulting from the formula (3.2) to have unusual dependencies and that this is so is seen from the following illustration:

$$\text{Let } x_{i+1} = 5x_i \pmod{m}$$

$$\text{Here } x_{i+1} = 5x_i - h_i m \quad (3.4)$$

in which h_i takes one of the values, 0, 1, 2, 3, 4. Thus pairs of successive values, (x_i, x_{i+1}) give the Cartesian co-ordinates of points which lie on just one of the five lines given by (3.4), and the larger m is, the longer the sequence of generated numbers will remain on any one of these lines before moving to another line. For example, if $x_0 = 1$, $m = 11$, then

$$x_1 = 5, x_2 = 3, x_3 = 4, x_4 = 9, x_5 = 1 \quad \checkmark$$

and the line used changes with each iteration.

However, if $x_0 = 1$, $m = 1000$, then

$$x_1 = 5, x_2 = 25, x_3 = 125, x_4 = 625, x_5 = 125 \quad \checkmark$$

and the sequence $x_1 \rightarrow x_4$ is obtained from the line

$$x_{i+1} = 5x_i \quad \checkmark$$

after which the sequence degenerates into a simple alternation pairs of successive values give points which lie on a limited number of straight lines, triplets of successive values lie on a limited number of planes, and so on (see Exercise 3.25).

The mixed congruential generator

$$x_{n+1} = 781x_n + 387 \pmod{1000} \quad (3.5) \quad \checkmark$$

has cycle length 1000. Figure 3.2 illustrates a plot of u_{n+1} vs. u_n for a sequence of length 500, where $u_i = x_i/1000$, for $0 \leq i \leq 499$.

The striking sparseness of the points is because of the small value of m used here; which also allows us to see very clearly the kind of pattern which can arise. Thus many users prefer to modify the output from congruential generators before use. One way to modify the output is to take numbers in groups of size g , say, and then 'shuffle' them, by means of a permutation, before use. The permutation used may be fixed, or chosen at random when required. Andrews *et al.* (1972) used such an approach with $g = 500$, while Egger (1979)

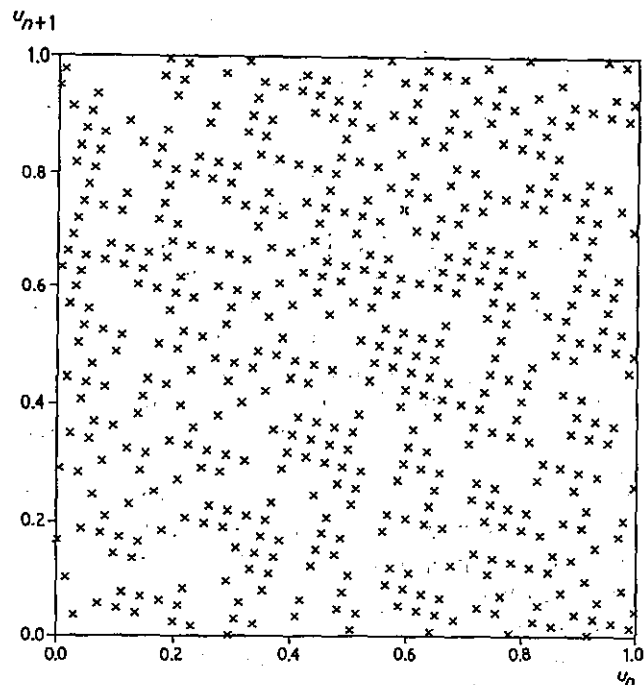


Figure 3.2 A plot of u_{n+1} vs. u_n for half the cycle of the mixed congruential generator of Equation (3.5).

used $g = 100$, a choice also investigated by Atkinson (1980). Page (1967) discusses the construction of random permutations, while tables of these are provided by Moses and Oakford (1963). See also the IMSL routine GGPER described in Appendix 1. An alternative approach, due to MacLaren and Marsaglia (1965) is to have a 'running' store of g numbers from a congruential generator, and to choose which of these numbers to use next by means of a random indicator digit from the range 1 to g , obtained, say, by a separate congruential generator. The gap in the store is then filled by the next number from the original generator, and so on. When this is done for the sequence resulting in Fig. 3.2, we obtain the plot of Fig. 3.3.

For further discussion, see Chambers (1977, p. 173) and Nance and Overstreet (1978). Nance and Overstreet discuss the value of g to be used, and conclude with Knuth (1981, p. 31) that for a good generator, shuffling is often not needed. On the other hand, shuffling can appreciably improve even very poor generators, as demonstrated by Atkinson (1980), a point which is also made in Exercise 3.26. The IMSL routine GGUW employs shuffling with $g = 128$; see Section A1.1 in Appendix 1.

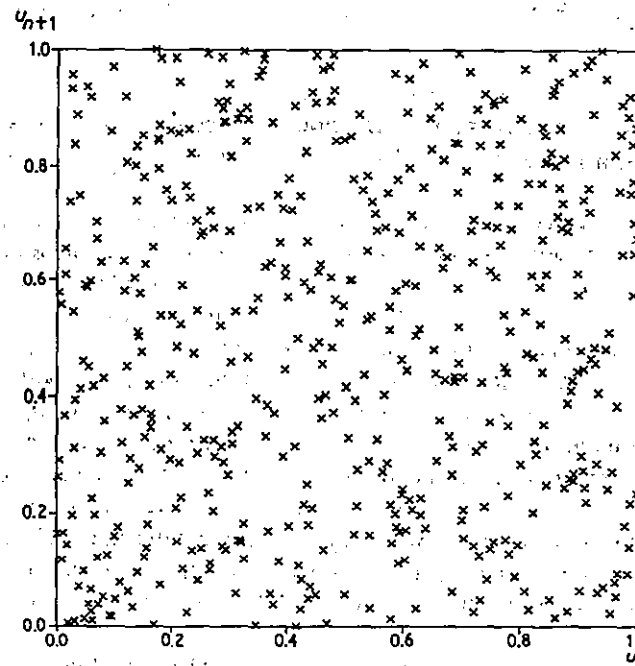


Figure 3.3 The plot resulting from modifying the same sequence that gave rise to Fig. 3.2. The modification entailed choosing the next number 'at random' from a store of length $g = 20$ of numbers from the original sequence, as explained in the text. In this example the random selection was made using Equation (3.1) and a seed of 0.5.

Successive digits in a decimal expansion of a truly random $U(0, 1)$ variable may, as we saw in Section 3.2, be used as uniform random digits. However, this approach is unwise in the case of pseudo-random $U(0, 1)$ variables because of the pattern effects which may arise (see the solution to Exercise 3.21). A disadvantage of congruential generators with $m = 2^k$ is that the low-order bits of generated numbers have short cycles (e.g. Atkinson, 1980). This is not a problem if m is prime (see Exercise 3.31) but then the arithmetic of the method is much more time-consuming on a 'binary' computer than if $m = 2^k$. Ways of reducing computational effort when m is prime are referenced by Law and Kelton (1982, p. 226).

3.7. Alternative methods of pseudo-random number generation

A variety of other methods of pseudo-random number generation exist—see for example, Andrews (1977, p. 170), O'Donovan (1979, p. 33), Law and Kelton (1982, p. 230), Tausworthe (1965) and Craddock and Farmer (1971). Miller and

Prentice (1968), for instance, use the third-order recurrence

$$x_j = x_{j-2} + x_{j-3} \pmod{p}$$

in which p is a suitable prime.

As with the congruential methods considered above, it is possible here also to examine the theoretical properties of the resulting sequence (cf. Exercise 3.26).

Different computers have different word-lengths (see Kennedy and Gentle 1980, p. 8), which determine the value of the modulus, m , used in congruential generators. This has resulted in machine-dependent generators, which is undesirable, as it makes it difficult to reproduce results, a positive feature of using pseudo-random numbers. Portable generators can result from representing 'large' integers by means of a number of 'short' word-length integers; see also Kral (1972) and Roberts (1982). An alternative approach is given by Wichmann and Hill (1982a, b), who combine three simple multiplicative congruential generators in such a way that the overall cycle-length is the product of the individual cycle lengths (see Exercises 3.17 and 3.18). The result is a portable generator with a cycle length greater than 2.78×10^{13} . As well as providing FORTRAN and Ada listings for their algorithm, they also provide an 82-step program for the Hewlett Packard HP-67 hand-calculator.

3.8 Summary and discussion

The building-blocks of simulation are $U(0,1)$ random variables, and random digits. We have seen that these may be obtained by the use of physical devices, or arithmetic formulae, and that no method is without its drawbacks. Large-scale simulations take place on computers, for which arithmetic formulae provide the most convenient approach. While any formula may seem to be adequate, and produce reasonable-looking numbers, there is always the danger that the formula could break down at some stage. The advantage of congruential generators is that they can be shown to possess certain desirable features; and to give guaranteed cycle lengths. There is always a chance, however, that because the numbers are pseudo-random, and not truly random, unwanted effects could still arise in any particular application. The answer is clearly to proceed with caution, and to make regular checks for oddities. Certain early generators were blatantly unsuitable, and the possibility remains that these generators are still in use. Well-used computer packages, such as MINITAB (see Ryan, Joiner and Ryan, 1976) do not always specify the generator they employ, which is clearly undesirable. (Indeed, different implementations of the same package may use different generators.) The same is true of certain widely used microcomputers. Possible pitfalls, as may occur here, can be avoided by the use of portable generators, which may be used on any machine, even a hand-calculator. Kennedy and Gentle (1980, p. 165) report that as many as about 30% of papers in the *Journal of the American Statistical Association* in 1978 employed simulation. In such a climate it is extremely

important for research papers to specify the algorithm used, and the tests for randomness employed in their investigation. At best, simulation results should be verified using a different generator.

In minimal BASIC there are two statements which relate to the work of this chapter. These are:

```
10 RANDOMIZE
20 U = RND
```

The first statement selects a seed in a random fashion, possibly by reference to the current time. If this statement is omitted, the pseudo-random number sequence that is used will always start from the same seed. In the second statement we obtain a realization of a pseudo-random $U(0,1)$ variable. Both of these statements will occur in programs in later chapters. While the BASIC instructions are as above, the underlying method used will vary from machine to machine, and on many microcomputers a slightly different form from RND is used.

The bibliographies by Sowey (1972, 1978) reveal that random number generation is a wide field of continuing interest. While new generators of proven improved properties may be developed in the future, congruential generators are likely to continue to prove popular and convenient. The need to test random numbers cannot be stressed too strongly, and this is a subject to which we shall return in Chapter 6. We shall now, in Chapters 4 and 5, proceed to see how uniform random numbers may be changed to give random variables of any kind.

*3.9 Proof of the attainment of a full cycle for a particular mixed congruential pseudo-random number generator

In the following, $a, b, c, k, s, t, \alpha, \gamma, \theta, \phi, h_1, h_2$ and h_3 denote positive integers.

THEOREM 3.1

The mixed congruential generator

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

with $a = 4c + 1$, b odd and $m = 2^k$, has cycle length m .

PROOF

The basis of the proof is to show that if $x_i = x_j$, for $i \neq j$, then we cannot have $|i - j| < m$. As the cycle length is $\leq m$, then this will prove that the cycle length is m , and the sequence generated within a single cycle is a permutation of the integers from 0 to $(m - 1)$. Without loss of generality, therefore, we shall take $x_0 = 0$, as this simplifies matters.

First of all, note that $x_n = y_n \pmod{m}$,

$$\text{where } y_{n+1} = ay_n + b, \quad \text{for } n \geq 0 \quad (3.6)$$

and, by the above, $y_0 = 0$.

From (3.6) we see that

$$y_n = b(1 + a + a^2 + \dots + a^{n-1}) \quad \text{for } n \geq 0$$

Now, $x_i = y_i - h_1 2^k$

and if $x_i = x_j$ for some $i > j$, say, then

$$b(a^i + a^{i+1} + \dots + a^{i-1}) = h_2 2^k$$

$$\text{i.e.,} \quad b a^j (1 + a + a^2 + \dots + a^{i-j-1}) = h_2 2^k \quad (3.7)$$

Let us write $w_n = 1 + a + \dots + a^{n-1}$ for $n \geq 1$.

In (3.7), by definition, a and b are odd, and so to prove the theorem we must show that:

$$w_{(i-j)} \neq h_3 2^k \quad \text{for } (i-j) < 2^k \quad (3.8)$$

and this we shall now do.

THE CASE $(i-j)$ ODD

If $(i-j)$ is odd, we can write $(i-j) = 2t+1$, say, for $t \geq 0$.

$$\begin{aligned} w_{2t+1} &= \left(\frac{1-a^{2t+1}}{1-a} \right) = \{(1+4c)^{2t+1} - 1\} / 4c \\ &= \{(1+4c)^t - 1\} \{(1+4c)^t + 1\} / 4c \\ &= \{(1+4c)^t + 1\} \left\{ \sum_{i=1}^t (4c)^{i-1} \binom{t}{i} \right\}, \end{aligned}$$

$$\text{which is even, as } 1 + (1+4c)^t = 2 + 4c \sum_{i=1}^t \binom{t}{i} (4c)^{i-1} \quad (3.9)$$

Thus $w_{2t+1} = w_{2t} + a^{2t+1}$ is odd, as a is odd, and so (3.8) is trivially true.

THE CASE $(i-j)$ EVEN

If $(i-j)$ is even, there exists an s such that $(i-j) = \alpha 2^s$, for some odd, positive integral α , and as $(i-j) < 2^k$, then $s < k$.

$$\begin{aligned} w_{(i-j)} &= w_{\alpha 2^s} = 1 + a + \dots + a^{\alpha 2^s - 1} = a^{\alpha 2^{s-1} - 1} + a^{\alpha 2^{s-1}} + \dots + a^{\alpha 2^s - 1} \\ &= w_{\alpha 2^{s-1}} + a^{\alpha 2^{s-1}} w_{\alpha 2^{s-1}} \\ &= w_{\alpha 2^{s-1}} (1 + a^{\alpha 2^{s-1}}) \\ &= w_{\alpha 2^{s-2}} (1 + a^{k_1}) (1 + a^{k_2}) \\ &\vdots \\ &= w_\alpha (1 + a^{k_1}) (1 + a^{k_2}) \dots (1 + a^{k_s}), \end{aligned} \quad (3.10)$$

for suitable positive integers, k_1, k_2, \dots, k_s .

Since $a = (1+4c)$, we have, from (3.9)

$$w_{\alpha 2^s} = w_\alpha \gamma 2^s,$$

in which w_α and γ are odd positive integers. (We have just proved that w_α is odd if α is odd.) Hence as $s < k$, there does not exist an h_3 such that

$$w_{\alpha 2^s} = h_3 2^k$$

This completes the proof. We note, finally, that it is simple to verify $x_0 = x_m$, since $(x_0 - x_m) = b w_m$, where $m = 2^k$, $w_2 = 1 + a = 2 + 4c$, so for $k = 1$, result (3.7) is true. Let us suppose that

$$w_m = \theta m, \quad \text{for } m = 2^k \text{ and } k \geq 1 \quad (3.11)$$

$$w_{2m} = \theta m (1 + a^m), \quad \text{from (3.10)}$$

and $(1 + a^m)$ is even, from (3.9).

Hence $w_{2m} = \phi(2m)$, and if (3.11) is true for $k \geq 1$, then it is also true for $(k+1)$. We have seen that it is true for $k = 1$, and so by induction it is true for all $k \geq 1$.

3.10 Exercises and complements

(a) Uses of random numbers

The randomized response technique (RRT) has been much studied and extended. A good introduction is provided by Campbell and Joiner (1973), who motivate the first four questions.

3.1 Investigate the workings of the RRT when the two alternative questions are:

- (i) I belong to group X;
- (ii) I do not belong to group X.

3.2 Describe how you would proceed if the proportion of positive responses to the RRT 'innocent' question is unknown. Can you suggest an innocent question for which it should be possible to obtain the proportion of correct responses without difficulty?

3.3 Investigate the RRT when the randomizing device is a bag of balls, each being one of three different colours, say red, white and blue, and the instructions to the (female) respondents are:

If the red ball is drawn answer the question: 'have you had an abortion'.

If the white ball is drawn, respond 'Yes'.

If the blue ball is drawn, respond 'No'.

- *3.4 In RRT, consider the implications for the respondent of responding 'Yes', even though it is not known which question has been answered. Consider how the technique might be extended to deal with frequency of activity. Consider how to construct a confidence interval (see, e.g., ABC, p. 266) for the estimated proportion.
- 3.5 100 numbered pebbles formed the population in a sampling experiment devised by J. M. Bremer. Students estimate the population mean weight ($\mu = 37.63$ g) by selecting 10 pebbles at random, using tables of random numbers, and additionally by choosing a sample of 10 pebbles, using their judgement only. The results obtained from a class of 32 biology undergraduates are given below:

Judgement sample means	Random sample means
62.63	31.45
35.85	32.12
55.36	51.93
66.43	24.74
34.96	43.32
37.23	29.41
34.45	42.67
60.53	47.94
49.61	28.76
56.07	56.43
59.02	31.21
50.65	32.73
33.34	55.37
58.62	36.65
47.02	22.44
48.34	40.04
28.56	44.65
26.65	41.43
46.34	39.39
27.86	26.39
39.62	23.88
25.45	35.15
48.82	35.88
66.56	28.03
37.25	31.71
45.98	43.98
32.46	61.49
54.03	31.52
51.89	33.99
62.81	33.78
59.74	49.69
14.05	22.97

Discuss, with reference to these data, the importance of taking random samples.

(b) On uniform random digits 8.023

- 3.6 A possible way of using two unbiased dice for simulating uniform random digits from 0 to 9 is as follows: throw the two dice and record the sum. Interpret 10 as 0, 11 as 1, and ignore 12. Discuss this procedure. (Based on part of an A-level examination question: Oxford, 1978.)
- 3.7 In Example 3.2 we used a fair coin to simulate events with probability different from 0.5. Here we consider the converse problem (the other side of the coin). Suppose you want to simulate an event with probability $\frac{1}{2}$; you have a coin but you suspect it is biased. How should you proceed? One approach is this: toss the coin twice. If the results of the two tosses are the same, repeat the experiment, and carry on like this until you obtain two tosses that are different. Record the outcome of the second toss. Explain why this procedure produces equi-probable outcomes. Discussion and extensions to this simple idea are given in Dwass (1972) and Hoeffding and Simons (1970).
- 3.8 In a series of 10 tosses of two distinguishable fair dice, A and B, the following faces were uppermost (A is given first in each case): (1, 4), (2, 6), (1, 5), (4, 3), (2, 2), (6, 3), (4, 5), (5, 1), (3, 4), (1, 2). Explain how you would use the dice to generate uniformly distributed random numbers in the range 0000–9999. (Based on part of an A-level examination question: Oxford, 1980.)
- 3.9 British car registration numbers are of the form: SHX 792R. Special rôles are played by the letters, but that is not, in general, true of the numbers. Collect 1000 digits from observing car numbers, and examine these digits for randomness (explain how you deal with numbers of the form: HCY 7F).
- 3.10 Below we give the decimal expansion of π to 2500 places, kindly supplied by T. Hopkins. Draw a bar-chart to represent the relative frequencies of some (if not all!) of these digits, and comment on the use of these digits as uniform random 0–9 digits. Note that Fisher and Yates (1948) adopted a not dissimilar approach, constructing random numbers from tables of logarithms; further discussion of their numbers is given in Exercise 6.8(ii).

3.1415926535 8979323846 2643383279 5028841971 6939937510
 5820974944 5923078164 0628620899 8628034825 3421170679
 8214808651 3282306647 0938446095 5058223172 5359408128
 4811174502 8410270193 8521105559 6448229489 5493038198
 4428810975 6659334461 2847564823 3786783165 2712019091
 4564856692 3460348610 4543266482 1339360728 0249141273
 7245870068 0631558817 4881520920 9828292540 9171536436
 7892590360 0113305305 4882046652 1384146951 9415116094
 3305727038 5759591953 0921861173 8193281179 3105118548
 0744623799 6274956735 1885752724 8912279381 8301194912

9833673362 4406566430 8602139494 6395224737 1907021798
 6094370277 0539217178 2931767523 8467481846 7669405132
 0005681271 4526356082 7785771342 7577896091 7869717872
 1468440901 2249534301 4654958537 1050792279 8892589235
 4201995611 2129021960 8640344181 5981362977 4771309960
 5187072113 4999999837 2978049951 0597317328 1609631859
 5024459455 3469083028 4252230825 3344685035 2819311881
 7101000313 7838752886 5875332083 8142081717 7669147303
 5982534904 2875546873 1159562863 8823597875 9375195778
 1857780532 1712268066 1300192787 6611195909 2164201989

3809525720 1065485863 2788659381 5338182796 8230301952
 0353018529 6899577362 2599413891 2497217752 8347913151
 5574857242 4541506959 5082953311 6881727855 8890750983
 8175463746 4939319255 0604009277 0167113900 9848824012
 8583616035 6370766010 4710181942 9555961989 4676783744
 9448255379 7747268471 0404753484 8208046684 2580694912
 9331367702 8989152104 7521620589 6602405803 8150193511
 2533824300 3558764024 7496473263 9141992726 0426992279
 6782354781 6360093417 2164121992 4586315030 2861829745
 5570674983 8505494588 5869269956 9092721079 7509302955

3211653449 8720275596 0236480665 4991198818 3479775356
 6369807426 5425278625 5181841757 4672890977 7727938000
 8164706001 6145249192 1732172147 7235014144 1973568548
 1613611573 5255213347 5741849468 4385233239 0739414333
 4547762416 8625189835 6948556209 9219222184 2725502542
 5688767179 0494601653 4668049886 2723279178 6085784383
 8279679766 8145410095 3883786360 9506800642 2512520511
 7392984896 0841284886 2694560424 1965285022 2106611863
 0674427862 2039194945 0471237137 8696095636 4371917287
 4677646575 7396241389 0865832645 9958133904 7802759009

9465764078 9512694683 9835259570 9825822620 5224894077
 2671947826 8482601476 9909026401 3639443745 5305068203
 4962524517 4939965143 1429809190 6592509372 2189648151
 5709858387 4105978859 5977297549 8930161753 8424681382
 6868386894 2774155991 8559252459 5395943104 9972524680
 8459872736 4469584865 3836736222 6260991246 0805124388
 4390451244 1365497627 8079771569 1435997700 1296180894
 4169486855 5848406353 4220722258 2848864815 8456028506
 0168427394 5226746767 8895252138 5225499546 6672782398

(c) On pseudo-random numbers

3.11 The first pseudo-random number generator was the 'mid-square' proposed by von Neumann (1951). The method is as follows: select a large integer, e.g. 7777. Square it and use the middle four digits as the next integer, square that, and so on. Here we get:

7777 → 60481729 → 4817 → 23203489 → 2034 → 4137156
 → 1371 → 1879641 → etc.

The above sequence illustrates how we proceed when the squared number does not fill the entire possible field-length of 8. Investigate and comment upon this procedure. Further discussion is provided by Tocher (1975, p. 72) and Knuth (1981, p. 3), who explain the problems that can arise with this method. Craddock and Farmer (1971) provide a modification which avoids the obvious degeneration when the process results in zero.

3.12 Investigate sequences produced by:

$$u_{n+1} = \text{fractional part of } (\pi + u_n)^5.$$

3.13 Show that for a full-period mixed congruential generator the mean and variance of the values produced by dividing each integer element in the full-period sequence by the modulus m are, respectively, $\frac{1}{2}(1 - 1/m)$, and $(1 + 1/m)/12$.

3.14 The following BASIC program simulates the mixed congruential generator of Equation (3.4), with $a = 781$, $b = 387$, $m = 1000$. Run this

```

10 REM MIXED CONGRUENTIAL GENERATOR
20 INPUT U0
30 LET A = 781
40 LET B = 387
50 FOR I = 1 TO 1000
60 LET U1 = (A*U0+B)/1000
70 LET U1 = (U1-INT(U1))*1000
80 LET U0 = U1
90 PRINT U1
100 NEXT I
110 END

```

program with and without the following change (from Cooke, Craven and Clarke, 1982, p. 70):

$$75 \quad U1 = \text{INT}(U1 + 0.5)$$

Comment on the results and the reason for using this additional line.

3.15 In pseudo-random number generation using congruential methods we obtain a sequence of integers $\{x_i\}$ over the range $(0, m)$. Approximations to $U(0, 1)$ random variables are then obtained by setting $u_i = x_i/m$. Show that

$$u_{i+1} = (au_i + b/m) \pmod{1}$$

and program this in BASIC (note the lesson of Exercise 3.14 with regard to round-off error). Note also the comments of Knuth (1981, p. 525).

- 3.16 Show that for a mixed congruential generator, with $a > 1$,

$$x_{n+k} = [a^k x_n + (a^k - 1)b/(a - 1)] \pmod{m} \quad \text{for } k \geq 0, n \geq 0$$

This property is useful in distributed array processing (DAP) programming of congruential generators (Sylwestrowicz, 1982).

- *3.17 Show that if U_1 and U_2 are independent $U(0, 1)$ random variables, then the fractional part of $(U_1 + U_2)$ is also $U(0, 1)$. Show further that this result still holds if U_1 is $U(0, 1)$, but U_2 has any continuous distribution.

- 3.18 (continuation) Show that if U_1, U_2 and U_3 are formed independently from congruential generators with respective cycle lengths c_1, c_2 and c_3 , then we may take the fractional part of $(U_1 + U_2 + U_3)$ as a realization of a pseudo-random $U(0, 1)$ random variable, and the resulting sequence of $(0, 1)$ variables will have cycle length $c_1 c_2 c_3$ if c_1, c_2 and c_3 are relatively prime. For further discussion, see Neave (1972, p. 6) and Wichmann and Hill (1982a).

- 3.19 In a mixed congruential generator, show that if $m = 10^k$ for some positive integer $k > 1$, then for the cycle length to equal m , we need to set $a = 20d + 1$, where d is a positive integer.

- 3.20 Show that the sequence $\{x_i\}$ of Section 3.5, for which $x_0 = 89, x_1 = 16$, etc., alternates between even and odd numbers.

- *3.21 (a) (Peach, 1961) The mixed congruential generator,

$$x_{n+1} = 9x_n + 13 \pmod{32}$$

has full (32) cycle length. Write down the resulting sequence of numbers and investigate it for patterns. For example, compare the numbers in the first half with those in the second half, write the numbers in binary form, etc.

- (b) Experiment with congruential generators of your own.

- 3.22 (a) Write BASIC programs to perform random shuffling and random replacement of pseudo-random numbers. When might these two procedures be equivalent?

- (b) (Bays and Durham, 1976) We may use the next number from a congruential generator to determine the random replacement. Investigate this procedure for the generator

$$x_{n+1} = 5x_n + 3 \pmod{16}; x_0 = 1.$$

- 3.23 A distinctly non-random feature of congruential pseudo-random numbers is that no number appears twice within a cycle. Suggest a simple procedure for overcoming this defect.

- 3.24 Construct a pseudo-random number generator of your own, and evaluate its performance.

- *3.25 The much-used IBM generator RANDU is multiplicative congruential, with multiplier 65 539, and modulus 2^{31} , so that the generated sequence is:

$$x_{i+1} = 65\,539x_i \pmod{2^{31}}$$

Use the identity $65\,539 = 2^{16} + 3$ to show that

$$x_{i+1} = (6x_i - 9x_{i-1}) \pmod{2^{31}},$$

and comment on the behaviour of successive triplets (x_{i-1}, x_i, x_{i+1}) . See also Chambers (1977, p. 191), Miller (1980a, b) and Kennedy and Gentle (1980, p. 149) for further discussion of this generator. Examples of plots of triplets are to be found in Knuth (1981, p. 90) and Oakenfull (1979).

- 3.26 (a) The Fibonacci series may be used for a pseudo-random number generator:

$$x_{n+1} = (x_n + x_{n-1}) \pmod{m}$$

Investigate the behaviour of numbers resulting from such a series. See Wall (1960) for an investigation of cycle-length when $m = 2^k$.

- (b) (Knuth, 1981) In a random sequence of numbers, $0 \leq x_i < m$, how often would you expect to obtain $x_{n-1} < x_{n+1} < x_n$? How often does this sequence occur with the generator of (a)? The Fibonacci series above is generally held to be a poor generator of pseudo-random numbers, but its performance can be much improved by shuffling (see Gebhardt, 1967). Oakenfull (1979) has obtained good results from the series

$$x_{n+1} = (x_n + x_{n-97}) \pmod{2^{35}}$$

Note that repeated numbers can occur with Fibonacci-type generators (cf. Exercise 3.23).

- 3.27 (a) For a multiplicative congruential generator, show that if a is an odd power of $8n \pm 3$, for any suitable integral n , and x_0 is odd, then all subsequent members of the congruential series are odd.

- (b) As we shall see in Chapter 5, it is sometimes necessary to form $\log_2 U$, where U is $U(0, 1)$. Use the result of (a) to explain the

advantage of such a multiplicative generator over a mixed congruential generator in such a case.

*3.28 Consider how you would write a FORTRAN program for a congruential generator.

*3.29 (Tausky and Todd, 1956) Consider the recurrence

$$y_{n+1} = y_n + y_{n-1} \quad \text{for } n \geq 1,$$

with $y_0 = 0, y_1 = 1$.

Show that

$$y_n = \left\{ \left(\frac{\sqrt{5}+1}{2} \right)^n - \left(\frac{1-\sqrt{5}}{2} \right)^n \right\} / \sqrt{5}$$

and deduce that for large n ,

$$y_n \approx \left(\frac{\sqrt{5}+1}{2} \right)^n / \sqrt{5}$$

Hence compare the Fibonacci series generator of Exercise 3.26 with a multiplicative congruential generator. Difference equations, such as that above, occur regularly in the theory of random walks (see Cox and Miller, 1965, Section 2.2).

3.30 The literature abounds with congruential generators. Discuss the choice of a, b, m , in the following. For further considerations, see Kennedy and Gentle (1980, p. 141) and Knuth (1981, p. 170).

(i) $\begin{matrix} a & b & m \\ 7^5 & 0 & 2^{31}-1 \end{matrix}$

Called GGL, this is IBM's replacement for RANDU (see Learmonth and Lewis, 1973). Egger (1979) used this generator in combination with shuffling from a $g = 100$ store, and it is the basis of routines GGUBFS and GGUBS of the IMSL library; see Section A1.1 in Appendix 1.

(ii) $\begin{matrix} a & b & m \\ 16333 & 25887 & 2^{15} \end{matrix}$ (from Oakenfull, 1979)

(iii) $\begin{matrix} a & b & m \\ 3432 & 6789 & 9973 \end{matrix}$ (see also Oakenfull, 1979)

(iv) $\begin{matrix} a & b & m \\ 23 & 0 & 10^8+1 \end{matrix}$ the Lehmer generator

This generator is of interest as it was the first proposed congruential generator, with $x_0 = 47\,594\,118$, by Lehmer (1951).

(v) The NAG generator: GOSCAF:

$$\begin{matrix} a & b & m \\ 13^{13} & 0 & 2^{59} \end{matrix}$$

See Section A1.1

(vi) $\begin{matrix} a & b & m \\ 171 & 0 & 30269 \end{matrix}$

This is one of the three component generators used by Wichmann and Hill (1982a, b).

(vii) $\begin{matrix} a & b & m \\ 131 & 0 & 2^{35} \end{matrix}$ used by Neave (1973).

(viii) $\begin{matrix} a & b & m \\ 2^7+1 & 1 & 2^{35} \end{matrix}$

This generator is of interest as it is one of the original mixed congruential generators, proposed by Rotenberg (1960).

(ix) $\begin{matrix} a & b & m \\ 397\,204\,094 & 0 & 2^{31}-1 \end{matrix}$

This is the routine GGUBT of the IMSL library—see Section A1.1

3.31 Show that the cycle length in a multiplicative congruential generator is given by the smallest positive integer n satisfying $a^n \equiv 1 \pmod{m}$. (See Exercise 3.16.)

We stated in Section 3.5, that if $m = 2^k$ in a multiplicative congruential generator, only one-quarter of the integers $0-m$ are obtained in the generator cycle. However, if m is a prime number then a cycle of length $(m-1)$ can be obtained with multiplicative congruential generators. Let $\phi(m)$ be the number of integers less than and prime to m , and suppose m is a prime number, p . Clearly, $\phi(p) = (p-1)$.

It has been shown (Tocher, 1975, p. 76) that the n above must divide $\phi(m)$. If $n = \phi(p)$ then a is called a 'primitive root' mod (p) , and the cycle length $(p-1)$ is attained. Ways of identifying primitive roots of prime moduli are given by Downham and Roberts (1967); for example, 2 is a primitive root of p if $(p-1)/2$ is prime and $p \equiv 3 \pmod{8}$. Given a primitive root r , then further primitive roots r may be generated from: $r = r^k \pmod{p}$, where k and $(p-1)$ are co-prime.

Use these results to verify that the following 5 prime modulus multiplicative congruential generators, considered by Downham and Roberts (1967), have cycle length $(p-1)$.

	$m = p$	a
(i)	67 101 323	8 192
(ii)	67 099 547	8 192
(iii)	16 775 723	32 768
(iv)	67 100 963	8
(v)	7 999 787	32

Extensions and further discussion are given by Knuth (1981, pp. 19–22) and Fuller (1976), while relevant tables are provided by Hauptman *et al.* (1970) and Western and Miller (1968).

- *3.32 If a fair coin is tossed until there are two consecutive heads, show that the probability that n tosses are required is

$$p_n = y_{n-1}/2^n \quad \text{for } n \geq 2$$

where the y_n are given by the Fibonacci numbers of Exercise 3.29 (cf. Exercise 3.26). We see from Exercise 3.29 that as $n \rightarrow \infty$, the ratio $y_n/y_{n-1} \rightarrow$ the golden ratio, $\phi = (1 + \sqrt{5})/2$, so that the tail of the distribution is approximately geometric, with parameter $\phi/2$. Mead and Stern (1973) suggest uses of this problem in the empirical teaching of statistics. Verify that the distribution above has mean 6.

4

PARTICULAR METHODS FOR NON-UNIFORM RANDOM VARIABLES

Some of the results of Chapter 2 may be used to convert uniform random variables into variables with other distributions. It is the aim of this chapter to provide some examples of such particular methods for simulating non-uniform random variables. Because of the important rôle played by the normal distribution in statistics, we shall start with normally distributed random variables.]

4.1 Using a central limit theorem

It is because of central limit theorems that the normal distribution is encountered so frequently, and forms the basis of much statistical theory. It makes sense, therefore, to use a central limit theorem in order to simulate normal random variables. For instance, we may simulate n independent $U(0, 1)$ random variables, U_1, U_2, \dots, U_n , say, and then set $N = \sum_{i=1}^n U_i$. As $n \rightarrow \infty$ the distribution of N tends to that of a normal variable. But in practice, of course, we settle on some finite value for n , so that the resulting N will only be approximately normal. So how large should we take n ? The case $n = 2$ is unsuitable, as N then has a triangular distribution (see Exercise 4.8), but for $n = 3$, the distribution of N is already nicely 'bell-shaped', as will be shown later. The answer to this question really depends on the use to which the resulting numbers are to be put, and how close an approximation is desired. [A convenient number to take is $n = 12$, since, as is easily verified, $E[U_i] = \frac{1}{2}$ and $\text{Var}[U_i] = 1/12$, so that then

$$N = \sum_{i=1}^{12} U_i - 6$$

is an approximately normal random variable with mean zero and unit variance. Values of $|N| > 6$ do not occur, which could, conceivably, be a problem for large-scale simulations. The obvious advantage of this approach, however, is

its simplicity; it is simple to understand, and simple to program, as we can see from Fig. 4.1.

```

10 RANDOMIZE
20 INPUT M
30 REM PROGRAM TO SIMULATE 2*M
40 REM APPROXIMATELY STANDARD
50 REM NORMAL RANDOM VARIABLES
60 REM USING A CENTRAL LIMIT
70 REM THEOREM APPROACH
80 FOR I = 1 TO 2*M
90 LET N = 0
100 FOR J = 1 TO 12
110 LET N = N+RND
120 NEXT J
130 PRINT N-6
140 NEXT I
150 END
    
```

Figure 4.1 BASIC programs for simulating 2M standard normal random variables.

4.2 The Box-Müller and Polar Marsaglia methods

4.2.1 The Box-Müller method

The last method used a convolution to provide approximately normal random variables. The next method we consider obtains exact normal random variables by means of a one-to-one transformation of two $U(0, 1)$ random variables. If U_1 and U_2 are two independent $U(0, 1)$ random variables then Box and Muller (1958) showed that

$$N_1 = (-2 \log_e U_1)^{1/2} \cos(2\pi U_2) \tag{4.1}$$

and $N_2 = (-2 \log_e U_1)^{1/2} \sin(2\pi U_2)$

are independent $N(0, 1)$ random variables.

At first sight this result seems quite remarkable, as well as most convenient. It is, however, a direct consequence of the result of Example 2.4, as we shall now see.

If we start with independent $N(0, 1)$ random variables, N_1 and N_2 , defining a point (N_1, N_2) in two dimensions by Cartesian co-ordinates, and we change to polar co-ordinates (R, Θ) , then

$$\begin{aligned} N_1 &= R \cos \Theta \\ N_2 &= R \sin \Theta \end{aligned} \tag{4.2}$$

and in Example 2.4 we have already proved that R and Θ are then independent random variables, Θ with a $U(0, 2\pi)$ distribution, and $R^2 = N_1^2 + N_2^2$ with a χ_2^2 distribution, i.e. an exponential distribution of mean 2. Furthermore, to

simulate Θ we need simply take $2\pi U_2$, where U_2 is $U(0, 1)$, and to simulate R we can take $(-2 \log_e U_1)$, where U_1 is $U(0, 1)$, as explained in Exercises 2.1 and 2.2.

We therefore see that Box and Müller have simply inverted the relationship of (4.2), which goes from (N_1, N_2) of a particular kind to (R, Θ) of a particular kind, and instead move from (R, Θ) to (N_1, N_2) , simulating Θ by means of $2\pi U_2$, and an independent R from $(-2 \log_e U_1)^{1/2}$, where U_1 is independent of U_2 . You are asked to provide a formal proof of (4.1) in Exercise 4.6. As we can see from Fig. 4.1, this method is also very easy to program, and each method considered so far would be easily operated on a hand-calculator.

If the Box-Müller method were to be used regularly on a computer then it would be worth incorporating the following interesting modification, which avoids the use of time-consuming sine and cosine functions.

*4.2.2 The Polar Marsaglia Method

The way to avoid using trigonometric functions is to construct the sines and cosines of uniformly distributed angles directly *without* first of all simulating the angles. This can be done by means of a rejection method as follows:

If U is $U(0, 1)$, then $2U$ is $U(0, 2)$, and $V = 2U - 1$ is $U(-1, 1)$.

If we select two independent $U(-1, 1)$ random variables, V_1 and V_2 , then these specify a point at random in the square of Fig. 4.2, with polar co-ordinates (\bar{R}, Θ) given by:

$$\bar{R}^2 = V_1^2 + V_2^2$$

and $\tan \Theta = V_2/V_1$

Repeated selection of such points provides a random scatter of points in the square, and rejection of points outside the inscribed circle shown leaves us with a uniform random scatter of points within the circle.

For any one of these points it is intuitively clear (see also Exercise 4.11) that the polar co-ordinates R and Θ are independent random variables, and further that Θ is a $U(0, 2\pi)$ random variable. In addition (see Exercise 4.11) \bar{R}^2 is $U(0, 1)$ and so the pair (\bar{R}, Θ) are what are required by the Box-Müller method, and we can here simply write

$$\sin \Theta = \frac{V_2}{\bar{R}} = V_2(V_1^2 + V_2^2)^{-1/2}$$

$$\cos \Theta = V_1(V_1^2 + V_2^2)^{-1/2}$$

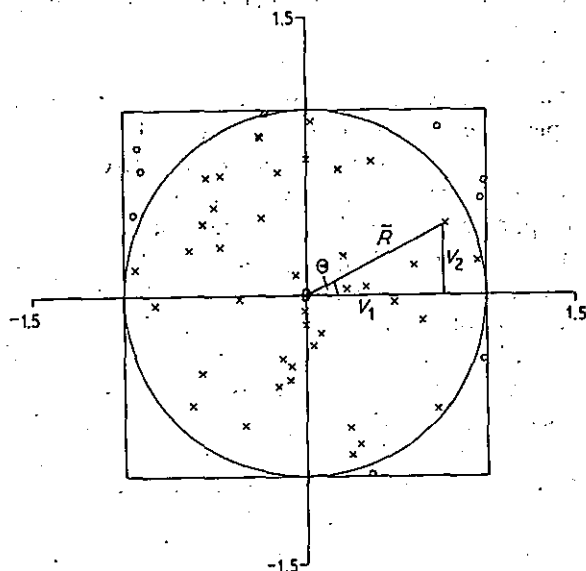


Figure 4.2 An illustration of points (denoted by \circ and \times) uniformly distributed over the square shown. The points denoted by \circ are rejected when one simply requires points uniformly distributed over the unit disc, as in the Polar Marsaglia method.

so that a pair of independent $N(0, 1)$ variables, N_1 and N_2 , are given by:

$$N_1 = (-2 \log(\bar{R}^2))^{1/2} V_2 (V_1^2 + V_2^2)^{-1/2}$$

$$N_2 = (-2 \log(\bar{R}^2))^{1/2} V_1 (V_1^2 + V_2^2)^{-1/2},$$

i.e.
$$N_1 = (-2 \log(V_1^2 + V_2^2))^{1/2} V_2 (V_1^2 + V_2^2)^{-1/2}$$

$$N_2 = (-2 \log(V_1^2 + V_2^2))^{1/2} V_1 (V_1^2 + V_2^2)^{-1/2}$$

resulting in

$$N_1 = V_2 \left(\frac{-2 \log W}{W} \right)^{1/2}$$

$$N_2 = V_1 \left(\frac{-2 \log W}{W} \right)^{1/2}$$

where $W = V_1^2 + V_2^2$.

The philosophy of rejection may seem rather strange at first, as it involves discarding variates obtained at a certain cost and effort, but pairs of variates

(V_1, V_2) are rejected just a proportion $1 - \pi/4$ of the time. The advantage of the rejection method here is that it provides a very simple way of obtaining a uniform scatter of points inside the circle of Fig. 4.2. Another rejection method was described in Example 3.2, and we shall encounter more general rejection methods in the next chapter, which have the same aim and use as here.

A BASIC program for this method is given in Fig. 4.3. Now known as the 'Polar Marsaglia' method, this approach is due originally to Marsaglia and Bray (1964), and is used in the IMSL routine GGNPM—see Section A1.1.

```

10 RANDOMIZE
20 INPUT M
30 REM PROGRAM TO SIMULATE 2*M STANDARD NORMAL
40 REM RANDOM VARIABLES USING THE POLAR
50 REM MARSAGLIA METHOD
60 FOR I = 1 TO M
70 LET V1 = 2*RND-1
80 LET V2 = 2*RND-1
90 LET R2 = V1*V1+V2*V2
100 IF R2 > 1 THEN 70
110 LET Y = SQR((-2*LOG(R2))/R2)
120 PRINT V1*Y,V2*Y
130 NEXT I
140 END

```

Figure 4.3 BASIC program for simulating $2M$ standard normal random variables, using the Polar Marsaglia method.

4.3 Exponential, gamma and chi-square variates

Random variables with exponential and gamma distributions are frequently used to model waiting times in queues of various kinds, and this is a natural consequence of the predictions of the Poisson process. The simplest way of obtaining random variables with an exponential p.d.f. of e^{-x} for $x \geq 0$ is to set $X = -\log_e U$, where U is $U(0, 1)$, as has already been done in the previous section (see Exercise 2.1).

We have also seen that $Y = X/\lambda$ has the exponential p.d.f. $\lambda e^{-\lambda x}$ for $x \geq 0$ (Exercise 2.2). An alternative approach for simulating exponential random variables will be given later in Exercise 5.35.

We have seen in Section 2.10 that if we have independent random variables, Y_1, \dots, Y_n with density function $\lambda e^{-\lambda x}$ for $x \geq 0$, then

$$G = \sum_{i=1}^n Y_i$$

has a gamma, $\Gamma(n, \lambda)$, distribution. Thus to simulate a $\Gamma(n, \lambda)$ random variable for integral n we can simply set

$$G = -\frac{1}{\lambda} \sum_{i=1}^n \log_e U_i$$

where U_1, \dots, U_n are independent $U(0, 1)$ random variables, i.e.

$$G = -\frac{1}{\lambda} \log_e \left(\prod_{i=1}^n U_i \right)$$

Now a random variable with a χ_m^2 distribution is simply a $\Gamma(m/2, \frac{1}{2})$ random variable (see Section 2.10), and so if m is even we can readily obtain a random variable with a χ_m^2 distribution, by the above approach. If m is odd, we can obtain a random variable with a χ_{m-1}^2 distribution by first obtaining a $\Gamma((m-1)/2, \frac{1}{2})$ random variable as above, and then adding to it N^2 , where N is an independent $N(0, 1)$ random variable (see Exercise 2.5). Here we are using the defining property of χ^2 random variables on integral degrees of freedom, and use of this property alone provides us with a χ_m^2 random variable from simply setting

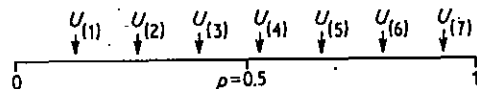
$$Z = \sum_{i=1}^m N_i^2 \tag{4.3}$$

where the N_i are independent, $N(0, 1)$ random variables. However, because of the time taken to simulate $N(0, 1)$ random variables, this last approach is not likely to be very efficient. Both NAG and IMSL computer packages use convolutions of exponential random variables in their routines for the generation of gamma and chi-square random variables (see Section A1.1). The simulation of gamma random variables with non-integral shape parameter, n , is discussed in Section 4.6.

4.4 Binomial and Poisson variates

4.4.1 Binomial variates

A binomial $B(n, p)$ random variable, X , can be written as $X = \sum_{i=1}^n B_i$, where the B_i are independent *Bernoulli* random variables, each taking the values, $B_i = 1$, with probability p , or $B_i = 0$, with probability $(1 - p)$. Thus to simulate such an X , we need just simulate n independent $U(0, 1)$ random variables, U_1, \dots, U_n , and set $B_i = 1$ if $U_i \leq p$, and $B_i = 0$ if $U_i > p$. The same end result can, however, be obtained from judicious re-use of a single $U(0, 1)$ random variable U . Such re-use of uniform variates is employed by the IMSL routine, GGBN when $n < 35$ (see Section A1.1). If $n \geq 35$, a method due to Relles (1972) is employed by this routine: in simulating a $B(n, p)$ variate we simply count how many of the U_i are less than p . If n is large then time can be saved by ordering the $\{U_i\}$ and then observing the location of p within the ordered sample. Thus if we denote the ordered sample by $\{U_{(i)}\}$, for the case $n = 7$, and $p = 0.5$ we might have:



In this example we would obtain $X = 3$ as a realization of a $B(7, \frac{1}{2})$ random variable.

Rather than explicitly order, one can check to see whether the sample median is greater than or less than p , and then concentrate on the number of sample values between p and the median. In the above illustration the sample median is $U_{(4)} > p$, and so we do not need to check whether $U_{(i)} > p$ for $i > 4$. However, we do not know, without checking, whether $U_{(i)} > p$ for any $i < 4$. This approach can clearly now be iterated by seeking the sample median of the sample: $(U_{(1)}, U_{(2)}, U_{(3)}, U_{(4)})$ in the above example, checking whether it is greater or less than p , etc. (see Exercise 4.18). A further short-cut results if one makes use of the fact that sample medians from $U(0, 1)$ samples can be simulated directly using a beta distribution (see Exercise 4.17). Full details are given by Relles (1972), who also provides a FORTRAN algorithm. An alternative approach, for particular values of p only, is as follows.

If we write U in binary form to n places, and if indeed U is $U(0, 1)$, then independently of all other places the i th place is 0 or 1 with probability $\frac{1}{2}$ (cf. Section 3.2). Thus, for example, if $U_1 = 0.10101011100101100$, we obtain 9 as a realization of a $B(17, \frac{1}{2})$ random variable, if we simply sum the number of ones. Here the binary places correspond to the trials of the binomial distribution.

If we want a $B(17, \frac{1}{4})$ random variable, we select further an independent $U(0, 1)$ random variable, U_2 , say. If $U_2 = 0.10101101100110101$, then place-by-place multiplication of the digits in U_1 and U_2 gives: 0.10101001100100100 , in which 1 occurs with probability $\frac{1}{4}$ at any place after the point. In this illustration we therefore obtain 7 as a realization of a $B(17, \frac{1}{4})$ random variable.

This approach can be used to provide $B(n, p)$ random variables, when we can find m and r so that $p = m2^{-r}$ (see Exercise 4.3). Most people are not very adept at binary arithmetic, but quite efficient algorithms could result from exploiting these ideas if machine-code programming could be used to utilize the binary nature of the arithmetic of most computers. However, as we have seen in Chapter 3, pseudo-random $U(0, 1)$ variables could exhibit undesirable patterns when expressed in binary form.

4.4.2 Poisson variates

Random variables with a Poisson distribution of parameter λ can be generated as a consequence of the following result.

Suppose $\{E_i, i \geq 1\}$ is a sequence of independent random variables, each with an exponential distribution, of density $\lambda e^{-\lambda x}$, for $x \geq 0$. Let $S_0 = 0$ and $S_k = \sum_{i=1}^k E_i$ for $k \geq 1$, so that, from Section 4.3, the S_k are $\Gamma(k, \lambda)$ random variables. Then the random variable K , defined implicitly by the inequalities $S_K \leq 1 < S_{K+1}$ has a Poisson distribution with parameter λ . In other words, we set $S_1 = E_1$, and if $1 < S_1$, then we set $K = 0$. If $S_1 \leq 1$, then we set $S_2 = E_1 + E_2$, and then if $S_2 > 1$, we set $K = 1$. If $S_2 \leq 1$, then we continue,

setting $S_3 = E_1 + E_2 + E_3$, and so on, so that we set $K = i$ when, and only when, $S_i \leq 1 < S_{i+1}$ for $i \geq 0$.

The BASIC program in Fig. 4.4 shows how easily this algorithm may be programmed, and may also help in demonstrating how it works. Note that we simulate

$$S_k = \sum_{i=1}^k E_i \quad \text{by} \quad S_k = -\frac{1}{\lambda} \log \left(\prod_{i=1}^k U_i \right)$$

```

10 RANDOMIZE
20 INPUT M,L
30 REM PROGRAM TO SIMULATE M RANDOM
40 REM VARIABLES FROM A POISSON
50 REM DISTRIBUTION OF PARAMETER L
60 LET E1 = EXP(-L)
70 FOR I = 1 TO M
80 LET K = 0
90 LET U = RND
100 IF U < E1 THEN 140
110 LET U = U * RND
120 LET K = K + 1
130 GOTO 100
140 PRINT K
150 NEXT I
160 END

```

Figure 4.4 BASIC program for simulating M Poisson random variables.

where as usual the U_i are independent $U(0, 1)$ random variables, as explained in Section 4.3. The comparison $S_k > 1$, then becomes

$$-\frac{1}{\lambda} \log \left(\prod_{i=1}^k U_i \right) > 1$$

i.e. $\log \left(\prod_{i=1}^k U_i \right) < -\lambda$ i.e. $\prod_{i=1}^k U_i < e^{-\lambda}$

and it is this inequality which is being tested in line number 100 of the program.

On first acquaintance, this algorithm has the same 'rabbit-out-of-a-hat' nature as the Box-Müller method. We can certainly show analytically that K , thus defined has the required Poisson distribution (see Exercise 4.9), but a consideration of the Poisson process, mentioned in Section 2.7, shows readily the origin of this algorithm, as we shall now see.

In a Poisson process in time (say) of rate λ we have the two important results (see, e.g., ABC, chapter 19):

- times between events are independent random variables from the exponential p.d.f., $\lambda e^{-\lambda x}$, for $x \geq 0$;
- the number of events in any fixed time interval of length t has a Poisson distribution of parameter (λt) .

Result (b) tells us that to simulate a random variable with a Poisson

distribution of parameter λ , all we have to do is construct a realization of a Poisson process of parameter λ , and then count the number of events occurring in a time interval of unit length. Result (a) tells us how we can simulate the desired Poisson process, by simply placing end-to-end independent realizations of exponential random variables from the $\lambda e^{-\lambda x}$ density. We keep a record of the time taken since the start of the process, and stop the simulation once that time exceeds unity. Figure 4.5 provides an illustration, resulting in $K = 3$, as there have been just three events in the Poisson process in the $(0, 1)$ time interval, occurring at times E_1 , $E_1 + E_2$ and $E_1 + E_2 + E_3$ respectively, with the fourth event occurring at time $E_1 + E_2 + E_3 + E_4 > 1$.

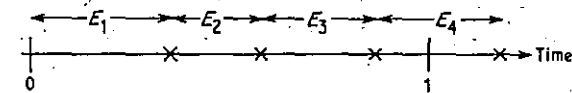


Figure 4.5 Illustration of the simulation of a Poisson process in time, starting at time 0. Four events occur, at times denoted by \times . Inter-event times, E_i , are independent random variables from the $\lambda e^{-\lambda x}$ exponential p.d.f., and the value $K = 3$, the number of events in the $(0, 1)$ time interval, is a realization of a random variable with a Poisson distribution of parameter λ .

*4.5 Multivariate random variables

Particular rules may also be exploited to simulate multivariate random variables. Two examples, one discrete and one continuous, will be considered here.

4.5.1 The bivariate Poisson distribution

This distribution was mentioned briefly in Section 2.16. If three independent random variables, X_1 , X_2 and X_3 , have Poisson distributions with parameters λ_1 , λ_2 and λ_3 respectively, then the derived variables $Y_1 = X_1 + X_3$, $Y_2 = X_2 + X_3$ have a bivariate Poisson distribution. This is readily verified by simply writing down the bivariate moment generating function for Y_1 and Y_2 , and observing it is of the form given in Equation (2.6). If we simulate X_1 , X_2 and X_3 by the method of Section 4.4.2 then this result readily allows us to simulate random variables Y_1 and Y_2 with a bivariate Poisson distribution. An alternative approach is suggested in Exercise 4.7.

4.5.2 The multivariate normal distribution

This distribution was discussed in Section 2.15. We saw there that if the p -variate random variable X has the multivariate normal, $N(0, I)$ distribution,

then $Z = AX + \mu$ has the multivariate normal $N(\mu, AA')$ distribution. Hence, if we want to simulate random variables from an $N(\mu, \Sigma)$ multivariate normal distribution, then we need only find a matrix A for which $\Sigma = AA'$. Ways of doing this are discussed in Exercise 4.14 and in the solution to that exercise. X is readily simulated, as its elements are independent and $N(0, 1)$. We then set $Z = AX + \mu$.

4.6 Discussion and further reading

We have seen in this chapter a utilization of formal relationships between random variables, which enables us to simulate a variety of random variables, using only $U(0, 1)$ variates; other illustrations can be found in the exercises. All of these examples are no more than useful tricks for particular cases. Often very simple algorithms result, as we have seen from some of the BASIC programs presented, and these algorithms could be readily implemented for small-scale simulations, using hand-calculators or microcomputers, for example. In a number of cases, however, the algorithms are less efficient than others which may be devised (see Kinderman and Ramage, 1976, for example), some of which will be considered in the next chapter.

The method of Section 4.4.2 for Poisson variates may become very inefficient if λ is large. In this case we would expect large numbers of events in the Poisson process during the $(0, 1)$ interval, resulting in prohibitively many checks. Atkinson (1979a) compares the algorithm of Section 4.4.2 for simulating Poisson random variables with alternative approaches which will be mentioned in the next chapter, while Kemp and Loukas (1978a, b) make similar comparisons for the bivariate Poisson case. More recent work for the univariate Poisson case is to be found in Atkinson (1979c), Kemp (1982), Ahrens and Dieter (1980, 1982) and Devroye (1981).

Atkinson and Pearce (1976), Atkinson (1977) and Cheng (1977) discuss the simulation of gamma $\Gamma(n, \lambda)$ random variables with non-integral shape parameter n , and we consider Cheng's method in Exercise 5.22. More recent work is provided by Cheng and Feast (1979) and Kinderman and Monahan (1980).

Neave (1973) showed that when the standard Box-Müller method is operated using pseudo-random numbers from a particular multiplicative-congruential generator, the resulting numbers exhibit some strikingly non-normal properties. This finding was taken up by Chay, Fardó and Mazumdar (1975) and Golder and Settle (1976), and we shall return to this point in Section 6.7.

We have in this chapter only scratched the surface of the relations between random variables of different kinds. The books by Johnson and Kotz (1969, 1970a, 1970b, 1972) provide many more such relationships, and the book by Mardia (1970) provides more information on bivariate distributions.

4.7 Exercises and complements

- 4.1 Show that a random variable with a $U(0, 1)$ distribution has mean $1/2$ and variance $1/12$.
- †4.2 Consider how you might simulate a binomial $B(3, p)$ random variable using just one $U(0, 1)$ variate, and write a BASIC program to do this.
- 4.3 Explain how the approach of using a binary representation of $U(0, 1)$ random variables may be used to simulate random variables with a binomial $B(n, p)$ distribution in which $p = m2^{-r}$, for integral $r > 0$, and integral $0 \leq m \leq 2^r$.
- 4.4 The following result is similar to one in Exercise 2.14: If the independent random variables X_1 and X_2 are, respectively, $\Gamma(p, 1)$ and $\Gamma(r, 1)$, then $Y = X_1/(X_1 + X_2)$ has the beta density,

$$f(y) = \frac{\Gamma(p+r)}{\Gamma(p)\Gamma(r)} y^{p-1} (1-y)^{r-1} \quad \text{for } 0 \leq y \leq 1$$

Use this result to write a BASIC program to simulate such a Y random variable, for integral $p > 1$ and $r > 1$.

- 4.5 If X_1, X_2, X_3, X_4 are independent $N(0, 1)$ random variables, we may use them to simulate other variates, using the results of Exercise 2.15 as follows:
- (a) $Y = |X_1 X_2 + X_3 X_4|$ has an exponential distribution of parameter 1.
- (b) $C = X_1/X_2$ has a Cauchy distribution, with density function $1/(\pi(1+x^2))$.

Use these results to write BASIC programs to simulate such Y and C random variables.

- †4.6 Prove that N_1, N_2 , given by Equation (4.1) are independent $N(0, 1)$ random variables.
- *4.7 When (X, Y) have a bivariate Poisson distribution, the probability generating function has the form

$$G(u, v) = \exp\{\lambda_1(u-1) + \lambda_2(v-1) + \lambda_3(uv-1)\}.$$

The marginal distribution of X is Poisson, of parameter $(\lambda_1 + \lambda_3)$, while the conditional distribution of $Y|X = x$ has probability generating function

$$\left(\frac{\lambda_1 + \lambda_3 v}{\lambda_1 + \lambda_3}\right)^x \exp[\lambda_2(v-1)]$$

Use these results to simulate the bivariate Poisson random variable (X, Y) .

- *4.8 If $X = \sum_{i=1}^n U_i$, where U_i are independent $U(0, 1)$ random variables, show, by induction or otherwise, that X has the probability density function

$$f(x) = \sum_{j=0}^{[x]} (-1)^j \binom{n}{j} (x-j)^{n-1} / (n-1)! \quad \text{for } 0 \leq x \leq n,$$

$$= 0 \quad \text{otherwise}$$

where $[x]$ denotes the integral part of x .

- *4.9 Prove, without reference to the Poisson process, that the random variable K , defined at the start of Section 4.4.2, has a Poisson distribution of parameter λ .
- *4.10 Consider how the Box-Muller method may be extended to more than two dimensions.
- *4.11 In the notation of the Polar Marsaglia method, show that Θ and R , defined by

$$\tan \Theta = V_1 / V_2 \quad \text{and} \quad R^2 = V_1^2 + V_2^2$$

both conditional on $V_1^2 + V_2^2 \leq 1$, are independent random variables. Show also that R^2 is a $U(0, 1)$ random variable, and Θ is a $U(0, 2\pi)$ random variable.

- *4.12 When a pair of variates (V_1, V_2) is rejected in the Polar Marsaglia method, it is tempting to try to improve on efficiency, and only reject one of the variates, so that the next pair for consideration would then be (V_2, V_3) , say. Show why this approach is unacceptable.
- *4.13 Provide an example of a continuous distribution, with density function $f(x)$, with zero mean, for which the following result is true: X_1 and X_2 are independent random variables with probability density function $f(x)$. When the point (X_1, X_2) , specified in terms of Cartesian co-ordinates, is expressed in polar co-ordinates (R, Θ) , then R, Θ are not independent.
- *4.14 If S is a square, symmetric matrix, show that it is possible to write $S = VDV'$, where D is a diagonal matrix, the i th diagonal element of which is the i th eigenvalue of S , and V is an orthogonal matrix with i th column an eigenvector corresponding to the i th eigenvalue of S . Hence provide a means of obtaining the factorization, $\Sigma = AA'$ required for the simulation of multivariate normal random variables in Section 4.5.2. More usually, a Choleski factorization is used for Σ , in which A is a lower-triangular matrix. Details are provided in the solution. This is the approach adopted in the IMSL routine GGNSM—see Section A1.1.

- *4.15 If X_1, X_2, \dots, X_n are independent (column) random variables from a p -variate multivariate normal, $N(0, \Sigma)$ distribution, then $Z = \sum_{i=1}^n X_i X_i'$ has the *Wishart* distribution, $W(Z; \Sigma; n)$, described, for example, by Press (1972, p. 100). Use this result, which generalizes to p dimensions the result of Equation (4.3), to provide a BASIC program to simulate such a Z . For related discussion, see Newman and Odell (1971, chapter 5).

- *4.16 If X_1, X_2 are independent $N(0, 1)$ random variables, show that the random variables X_1 and

$$Y_1 = \rho X_1 + (1 - \rho^2)^{1/2} X_2 \quad \text{where} \quad -1 \leq \rho \leq +1$$

have a bivariate normal distribution, with zero means, unit variances, and correlation coefficient ρ .

- *4.17 Let $U_1, U_2, \dots, U_{2n-1}$ be a random sample from the $U(0, 1)$ density. If M denotes the sample median, show that M has the $B_e(n, n)$ distribution.

- *4.18 (continuation) Consider how the result of Exercise 4.17 may be used to simulate a $B(n, p)$ random variable (Relles, 1972).

- *4.19 We find, from Section A1.1, that the IMSL computer library has routine GGPN for simulating Poisson variables when the Poisson parameter λ may vary from call to call. Otherwise one might use the IMSL routine GGPOS. Kemp (1982) was also concerned with Poisson variable simulation when λ may vary, and one might wonder why one should want to simulate such Poisson variates. An answer is provided by the following exercise.

The random variable X has the conditional Poisson distribution:

$$\Pr(X = k | \lambda) = \frac{e^{-\lambda} \lambda^k}{k!} \quad \text{for } k \geq 0$$

If λ has a $\Gamma(n, \theta)$ distribution, show that the unconditional distribution of X is

$$\Pr(X = k) = \binom{n+k-1}{k} \left(\frac{1}{\theta+1} \right)^k \left(\frac{\theta}{\theta+1} \right)^n \quad \text{for } k \geq 0$$

i.e. $X = Y - n$, where Y has a negative-binomial distribution as defined in Section 2.6. As $n \rightarrow 0$ the distribution tends to the logarithmic series distribution much used in ecology, and generalized by Kempton (1975). Kemp (1981) considers simulation from this distribution (see Exercise 4.22).

- 4.20 (continuation) Use the result of the last question to provide a BASIC

program to simulate negative-binomial random variables, for integral $n > 1$. This result is sometimes used to explain the frequent use of the negative-binomial distribution for describing discrete data when the Poisson distribution is unsatisfactory. The negative-binomial is a 'contagious' distribution, and much more relevant material is provided by Douglas (1980). An algorithm using the waiting-time definition of the distribution is given in the IMSL routine GGBNR (see Appendix 1).

- 4.21 Use the transformation theory of Section 2.12 to show that the random variable $Y = e^X$, where X has a $N(\mu, \sigma^2)$ distribution, has the density function

$$f_Y(y) = \frac{1}{y\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{\log_e(y) - \mu}{\sigma}\right)^2\right) \quad \text{for } y \geq 0$$

Y is said to have a *log-normal* distribution. The p.d.f. has the same qualitative shape as that of the $\Gamma(2, 1)$ p.d.f. of Fig. 2.6, and the log-normal distribution is often used to describe incubation periods for diseases (see also Morgan and Watts, 1980) and sojourn times in more general states. We shall, in fact, encounter such a use for this distribution in Example 8.3. Section A1.1 gives IMSL and NAG routines for simulating from this distribution. For full details, see Aitchison and Brown (1966).

- 4.22 (Kemp, 1981) The general logarithmic distribution is

$$p_k = -\alpha^k / \{k \log_e(1 - \alpha)\} \quad k \geq 1, 0 < \alpha < 1$$

Show that its moment generating function is:

$$\log(1 - \alpha e^t) / \log(1 - \alpha)$$

and that successive probabilities can be generated from:

$$p_k = \alpha(1 - 1/k)p_{k-1} \quad \text{for } k \geq 2$$

Show that if X has the conditional geometric distribution

$$\Pr(X = x | Y = y) = (1 - y)y^{x-1} \quad \text{for } x \geq 1$$

and if $\Pr(Y \leq y) = \frac{\log(1 - y)}{\log(1 - \alpha)}$ for $0 \leq y \leq \alpha$

then X has the logarithmic distribution. Explain how you can make use of this result to simulate from the logarithmic distribution.

5

GENERAL METHODS FOR NON-UNIFORM RANDOM VARIABLES

For many uses, simple algorithms, such as those which may arise from particular methods of the kind described in the last chapter, will suffice. It is of interest, however, to consider also *general* methods, which may be used for any distribution, and that we shall now do. In many cases general methods can result in algorithms which, while they are more complicated than those considered so far, are appreciably more efficient.

5.1 The 'table-look-up' method for discrete random variables

For ease of notation, let us suppose that we have a random variable X that takes the values 0, 1, 2, 3, etc., and with $p_i = \Pr(X = i)$ for $i \geq 0$. Thus X could be binomial, or Poisson, for example.

A general algorithm for simulating X is as follows:

Select a $U(0, 1)$ random variable, U .

Set $X = 0$ if $0 \leq U < p_0$, and

set $X = j$ if $\sum_{i=0}^{j-1} p_i \leq U < \sum_{i=0}^j p_i$ for $j \geq 1$.

We can think of the probabilities $\{p_i, i \geq 0\}$ being put end-to-end and, as $\sum_{i=0}^{\infty} p_i = 1$, filling out the interval $[0, 1]$ as illustrated in Fig. 5.1. We can now see that the above algorithm works by selecting a value U and observing in which probability interval U lands. In the illustration of Fig. 5.1 we have

$$\sum_{i=0}^1 p_i \leq U < \sum_{i=0}^2 p_i$$

and so we set $X = 2$.

This algorithm is simply a generalization to more than two intervals of the rule used to simulate Bernoulli random variables in Section 4.4.1. The

program to simulate negative-binomial random variables, for integral $n > 1$. This result is sometimes used to explain the frequent use of the negative-binomial distribution for describing discrete data when the Poisson distribution is unsatisfactory. The negative-binomial is a 'contagious' distribution, and much more relevant material is provided by Douglas (1980). An algorithm using the waiting-time definition of the distribution is given in the IMSL routine GGBNR (see Appendix 1).

- 4.21 Use the transformation theory of Section 2.12 to show that the random variable $Y = e^X$, where X has a $N(\mu, \sigma^2)$ distribution, has the density function

$$f_Y(y) = \frac{1}{y\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{\log_e(y) - \mu}{\sigma}\right)^2\right) \quad \text{for } y \geq 0$$

Y is said to have a *log-normal* distribution. The p.d.f. has the same qualitative shape as that of the $\Gamma(2, 1)$ p.d.f. of Fig. 2.6, and the log-normal distribution is often used to describe incubation periods for diseases (see also Morgan and Watts, 1980) and sojourn times in more general states. We shall, in fact, encounter such a use for this distribution in Example 8.3. Section A1.1 gives IMSL and NAG routines for simulating from this distribution. For full details, see Aitchison and Brown (1966).

- 4.22 (Kemp, 1981) The general logarithmic distribution is

$$p_k = -\alpha^k / \{k \log_e(1 - \alpha)\} \quad k \geq 1, 0 < \alpha < 1$$

Show that its moment generating function is:

$$\log(1 - \alpha e^t) / \log(1 - \alpha)$$

and that successive probabilities can be generated from:

$$p_k = \alpha(1 - 1/k)p_{k-1} \quad \text{for } k \geq 2$$

Show that if X has the conditional geometric distribution

$$\Pr(X = x | Y = y) = (1 - y)y^{x-1} \quad \text{for } x \geq 1$$

and if $\Pr(Y \leq y) = \frac{\log(1 - y)}{\log(1 - \alpha)}$ for $0 \leq y \leq \alpha$

then X has the logarithmic distribution. Explain how you can make use of this result to simulate from the logarithmic distribution.

5

GENERAL METHODS FOR NON-UNIFORM RANDOM VARIABLES

For many uses, simple algorithms, such as those which may arise from particular methods of the kind described in the last chapter, will suffice. It is of interest, however, to consider also *general* methods, which may be used for any distribution, and that we shall now do. In many cases general methods can result in algorithms which, while they are more complicated than those considered so far, are appreciably more efficient.

5.1 The 'table-look-up' method for discrete random variables

For ease of notation, let us suppose that we have a random variable X that takes the values 0, 1, 2, 3, etc., and with $p_i = \Pr(X = i)$ for $i \geq 0$. Thus X could be binomial, or Poisson, for example.

A general algorithm for simulating X is as follows:

Select a $U(0, 1)$ random variable, U .

Set $X = 0$ if $0 \leq U < p_0$, and

set $X = j$ if $\sum_{i=0}^{j-1} p_i \leq U < \sum_{i=0}^j p_i$ for $j \geq 1$.

We can think of the probabilities $\{p_i, i \geq 0\}$ being put end-to-end and, as $\sum_{i=0}^{\infty} p_i = 1$, filling out the interval $[0, 1]$ as illustrated in Fig. 5.1. We can now see that the above algorithm works by selecting a value U and observing in which probability interval U lands. In the illustration of Fig. 5.1 we have

$$\sum_{i=0}^1 p_i \leq U < \sum_{i=0}^2 p_i$$

and so we set $X = 2$.

This algorithm is simply a generalization to more than two intervals of the rule used to simulate Bernoulli random variables in Section 4.4.1. The

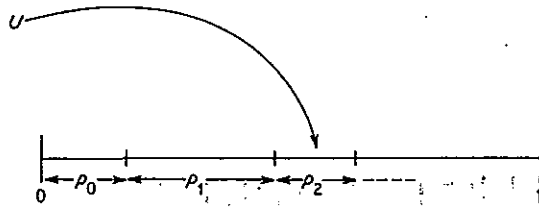


Figure 5.1 An illustration of how the table-look-up method works for simulating a discrete random variable with probability distribution $\{P_i, i \geq 0\}$.

reason the algorithm works is readily explained. We want to simulate the random variable X so that $\Pr(X = i) = p_i$ for $i \geq 0$. As U is $U(0, 1)$, then for any $0 \leq a \leq b$, $\Pr(a \leq U < b) = (b - a)$ (see Section 2.8) and so $\Pr(0 \leq U < p_0) = p_0 = \Pr(X = 0)$, and

$$\Pr\left(\sum_{i=0}^{j-1} p_i \leq U < \sum_{i=0}^j p_i\right) = p_j = \Pr(X = j) \quad \text{for } j \geq 1$$

Thus, for $j \geq 0$, the algorithm returns the value $X = j$ with probability p_j , as required.

The above algorithm is readily modified to cope with discrete random variables with different ranges from that considered above, (i.e. $X \geq 0$) and one such example now follows.

EXAMPLE 5.1

We want to simulate the geometric random variable X , with distribution

$$p_i = \Pr(X = i) = (1 - p)^{i-1} p \quad \text{for } i \geq 1, 0 < p < 1$$

In order to operate the above algorithm we need successive cumulative sums of the $\{p_i\}$, and in this case, because p_i is of a simple geometric form, then these cumulative sums are also of a simple form. Here,

$$\sum_{i=1}^j p_i = \frac{p(1 - (1 - p)^j)}{1 - (1 - p)} = 1 - (1 - p)^j \quad \text{for } j \geq 1$$

Thus the algorithm becomes:

$$\text{Set } X = j \text{ if } 1 - (1 - p)^{j-1} \leq U < 1 - (1 - p)^j \quad \text{for } j \geq 1$$

$$\text{which is equivalent to: } -(1 - p)^{j-1} \leq U - 1 < -(1 - p)^j$$

$$\text{i.e. } (1 - p)^{j-1} \geq (1 - U) > (1 - p)^j \quad (5.1)$$

Before proceeding, we can here observe that the algorithm entails selecting a $U(0, 1)$ random variable, and then checking the range of $(1 - U)$. Now it is intuitively clear that if U is a $U(0, 1)$ random variable, then so is $(1 - U)$, and

this result can be readily verified by the change-of-variable theory of Section 2.12 (see Exercise 5.1).

Hence we can reduce the labour of arithmetic slightly if we replace (5.1) by the equivalent test:

$$(1 - p)^{j-1} \geq U > (1 - p)^j \quad (5.2)$$

Of course, for any particular realization of U , (5.1) and (5.2) will usually give different results; however, the random variable X resulting from using (5.2) will have the same geometric distribution as the random variable resulting from using (5.1). Continuing from (5.2), we set $X = j \geq 1$ if, and only if,

$$(j - 1) \log_e(1 - p) \geq \log_e U > j \log_e(1 - p)$$

so that, recalling that $\log_e(1 - p) < 0$, we have $X = j$ if

$$(j - 1) \leq \frac{\log_e U}{\log_e(1 - p)} < j \quad \text{for } j \geq 1 \quad (5.3)$$

Finally, we note that we can express (5.3) very simply by setting

$$X = 1 + \left[\frac{\log_e U}{\log_e(1 - p)} \right] \quad (5.4)$$

where $[y]$ is used to denote the integral part of y . For further discussion of this result, see Exercise 5.12.

This example therefore uses the general table-look-up algorithm to produce the simple expression of (5.4). This is in contrast to a particular approach which may be used, based upon the definition of the geometric distribution given in Section 2.6. Thus an alternative method would be to test sequentially independent $U(0, 1)$ random variables until one was found to be less than p , and an algorithm using this approach is provided by the IMSL routine GGEO (see Section A1.1).

This example is unusual in that the cumulative sums of probabilities have a simple form. The next example is far more typical.

EXAMPLE 5.2

If X has a Poisson distribution of parameter 2, its cumulative distribution function is given below to four places of decimals:

i	0	1	2	3	4	5	6	7	8	9
$\Pr(X \leq i)$	0.1353	0.4060	0.6767	0.8571	0.9473	0.9834	0.9955	0.9989	0.9998	1.000

Using this table and the table-look-up algorithm, the following eight $U(0, 1)$

random variables can be seen to give rise to the indicated values of X :

U	X
0.0318	0
0.4167	2
0.4908	2
0.2459	1
0.3643	1
0.8124	3
0.9673	5
0.1254	0

This example illustrates why the table-look-up method is so called. Given a table of the cumulative distribution of any discrete random variable, and a supply of $U(0, 1)$ random variables, we can use this method to simulate that random variable. By their very nature, such tables are finite, and if the random variable in question has an infinite range, then the range would have to be truncated for the method to be used. This was done in the above example, where using accuracy of only four decimal places resulted in the range of X being truncated to $[0, 9]$.

Human beings can operate the table-look-up method quite easily, but its implementation on a computer poses some intriguing problems. First of all we can remark that for a computer implementation it is not necessary to store cumulative sums of probabilities—they can be computed each time, as required. Random variables of infinite range need not then have their range truncated, but this approach is usually far too costly in effort because of the repeated duplication of arithmetic each time a new simulation is run. More usually ranges are truncated if necessary, and the resulting finite tables are stored within the computer. The next problem that arises is how to read such stored tables. Computers need specified algorithms which could, for instance, involve reading the table of the cumulative distribution in Example 5.2 from left to right. In such a case, the computer would return $X = 0$ when $U = 0.0318$, with the greatest of ease; but when $U = 0.9673$ it would laboriously check whether $U < 0.1353$, $U < 0.4060$, and so on until it found $0.9473 < U < 0.9834$. Human beings need not be so rigid and have the advantage over computers of being able to change their strategy in the light of superficial evidence on the size of U . By analogy, when looking up a word such as 'wombat' in the dictionary, not many of us would start at the front, with the letter 'A' and then skim through from A to W; rather, we would start from the middle, or somewhere near the end, possibly even working backwards as well as forwards. A more efficient computer algorithm may result if the range of X

were initially subdivided; for example, if $\Pr(X \leq \theta) = p \approx 0.5$, say, for some known θ , then if $U > p$ it would not be necessary to check U against $\sum_{i=0}^j p_i$ for $j \leq \theta$. Such an approach is utilized in the IMSL routine GGDT and the NAG routine GO5EYF (see Section A1.1) and was encountered earlier in Section 4.4.1.

5.2 The 'table-look-up', or inversion method for continuous random variables

We shall now consider the analogue of the above method for continuous random variables. Suppose we wish to simulate a continuous random variable X with cumulative distribution function $F(x)$, i.e. $F(x) = \Pr(X \leq x)$, and suppose also that the inverse function, $F^{-1}(u)$ is well-defined for $0 \leq u \leq 1$.

If U is a $U(0, 1)$ random variable, then $X = F^{-1}(U)$ has the required distribution. We can see this as follows:

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

$$\text{then } \Pr(X \leq x) = \Pr(F^{-1}(U) \leq x)$$

and because $F(x)$ is the cumulative distribution function of a continuous random variable, $F(x)$ is a strictly monotonic increasing continuous function of x . This fact enables us to write

$$\Pr(F^{-1}(U) \leq x) = \Pr(U \leq F(x))$$

But, as U is a $U(0, 1)$ random variable,

$$\Pr(U \leq F(x)) = F(x) \quad (\text{see Section 2.8})$$

$$\text{i.e. } \Pr(X \leq x) = F(x)$$

and so the X obtained by setting $X = F^{-1}(U)$ has the required distribution.

The above argument, which was given earlier in Equation (2.1), is perhaps best understood by considering a few examples. Figure 5.2 illustrates one cumulative distribution function for a truncated exponential random variable. We operate the rule $X = F^{-1}(U)$ by simply taking values of $U(0, 1)$ variates and projecting down on the x -axis as shown, using the graph of $y = F(x)$.

We shall now consider two further examples in more detail.

EXAMPLE 5.3

In the untruncated form, if X has an exponential density with parameter λ , then

$$f(x) = \lambda e^{-\lambda x} \quad \text{for } x \geq 0, \lambda > 0,$$

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

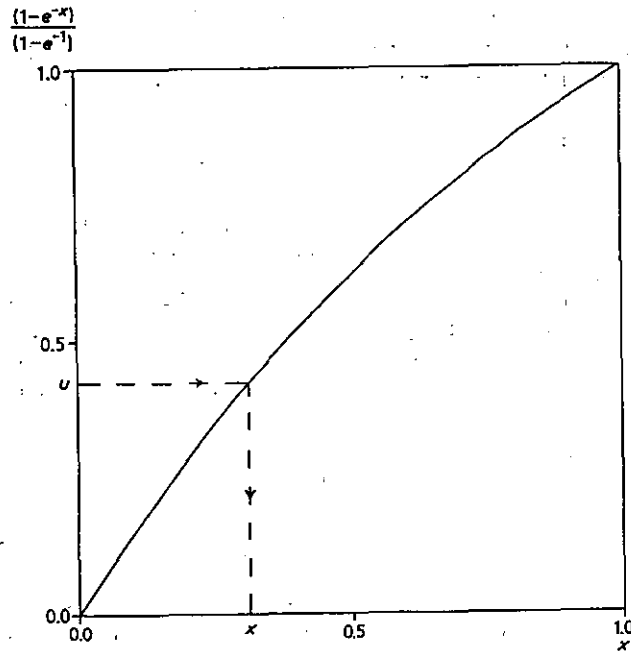


Figure 5.2 Operation of the table-look-up method for a continuous random variable. The curve has the equation $(1 - e^{-x})/(1 - e^{-1})$ and is the cumulative distribution function of a truncated exponential random variable, with probability density function, $e^{1-x}(e-1)^{-1}$ for $0 \leq x \leq 1$.

To simulate X we set $X = F^{-1}(U)$, i.e., set $U = F(X)$

$$U = 1 - e^{-\lambda x}, \text{ and solve for } X.$$

This gives $X = -\frac{1}{\lambda} \log_e(1 - U)$

and for the same reasoning as in Example 5.1, we obtain the desired distribution for X from setting

$$X = -\frac{1}{\lambda} \log_e U \quad (5.5)$$

A verification of this result is provided by the solution to Exercise 2.1, and this method is used in the IMSL routine GGEXN and the NAG routine GO5DBF (see Section A1.1).

As with Example 5.1, the result of (5.5) is deceptive in its simplicity, and it is no coincidence that the geometric and exponential distributions play similar

rôles, the former in the discrete case and the latter in the continuous case, as discussed in Section 2.10, Exercise 2.23 and Exercise 5.12. It is unfortunately the case that it is often *not* simple to form $X = F^{-1}(U)$. The prime example of this occurs with the normal distribution, which has led to a variety of different approximations to both the normal cumulative distribution function and its inverse. We shall return to the subject of these approximations later in Section 5.7 and Exercise 5.9.

We conclude this section with an example of how this method can be used, in a 'table-look-up' fashion to simulate standard normal random variables.

EXAMPLE 5.4

If we take the same $U(0, 1)$ values as in Example 5.2 then we can use tables of the standard normal cumulative distribution function, $\Phi(x)$ to give the following realizations of an $N(0, 1)$ random variable X :

U	X (to two places of decimals)
0.0318	-1.85
0.4167	-0.21
0.4908	-0.02
0.2459	-0.69
0.3643	-0.35
0.8124	0.89
0.9673	1.84
0.1254	-1.15

Thus, for example, $0.8124 = \Phi(0.89)$, to the accuracy given.

Two points should be made here:

- (a) Because of the symmetry of the $N(0, 1)$ distribution, the tables usually only give values of $x \geq 0$ and, correspondingly, values of $\Phi(x) \geq 0.5$, and so when $u < 0.5$ we have to employ the following approach which is easily verified to be correct:

We want x for which $u = \Phi(x)$.

If $u < 0.5$, then by the symmetry of the normal density, $x = -\Phi^{-1}(1 - u)$.

- (b) The accuracy of the numbers produced (in this case to two decimal places) depends on the accuracy of the tables, which also determines the degree of the truncation involved.

The 'table-look-up' method for continuous random variables is often called the *inversion method*, and a general algorithm is provided by the IMSL routine GGVCB (see Section A1.1). We shall use these terms interchangeably, though strictly they describe different ways of implementing the same basic method.

5.3 The rejection method for continuous random variables

Suppose we have a method for sprinkling points uniformly at random under any probability density function $f(x)$, and which may give rise to the pattern of points in Fig. 5.3. What is the probability that the abscissa, X say, of any one of these points lies in the range $\alpha \leq X < \beta$, for any $\alpha < \beta$?

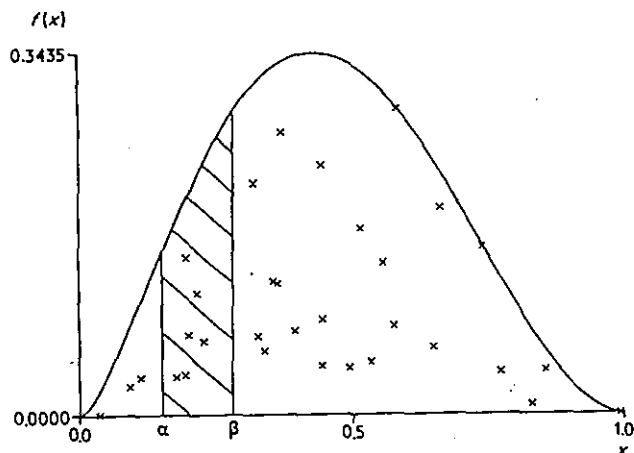


Figure 5.3 An illustration of points \times uniformly and randomly distributed underneath the probability density function $f(x)$. For illustration we have used the $B_c(2.5, 3)$ distribution.

The event, $\alpha \leq X < \beta$ is equivalent to the point being in the shaded area shown in Fig. 5.3, and so, because of the assumed uniform distribution of the points, this event has probability

$$\frac{\text{area of shaded area}}{\text{total area under } f(x)}$$

This is

$$\int_{\alpha}^{\beta} f(x) dx / \int_{-\infty}^{\infty} f(x) dx$$

i.e.

$$\int_{\alpha}^{\beta} f(x) dx \text{ as } \int_{-\infty}^{\infty} f(x) dx = 1,$$

since $f(x)$ is a probability density function.

Thus we are saying that

$$\Pr(\alpha \leq X < \beta) = \int_{\alpha}^{\beta} f(x) dx, \quad \text{for any } \alpha < \beta$$

where $f(x)$ is a probability density function, i.e. X has probability density function $f(x)$ (see Section 2.3).

Thus, for any probability density function $f(x)$, we can simulate random variables X from this density function as long as we have a method for uniformly and randomly sprinkling points under $f(x)$. Those who Section 4.2.2 will have already encountered a similar situation, being in that case to enclose within a square the area to be sprinkled. It is a simple matter to distribute points uniformly at random over a square, and in Section 4.2.2, those points not within the area of interest are rejected. The same principle for any density function $f(x)$ results in the rejection method, attributed to von Neumann (1951). While the rejection method (sometimes also called the 'acceptance-rejection' method) may be used for discrete random variables (see Fishman, 1979, for example), it is usually employed for continuous random variables, the case being investigated here.

If the probability density function $f(x)$ is non-zero over only a finite range, then it is easy to box it in, as shown in Fig. 5.4. Using $U(0, 1)$ random variables it is a simple matter to sprinkle points uniformly and randomly over the rectangle shown, simply by taking points with Cartesian co-ordinates $(\theta + (\alpha - \theta)U_1, \delta U_2)$, where U_1 and U_2 are independent $U(0, 1)$ random variables. Points landing above $f(x)$ are rejected, while for points landing below $f(x)$, we take $\theta + (\alpha - \theta)U_1$ as a realization of X .

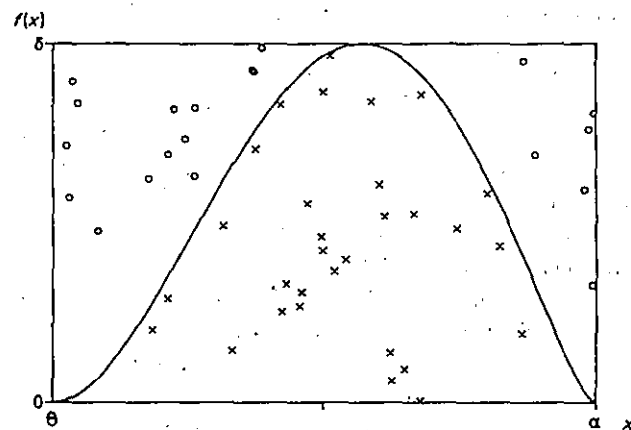


Figure 5.4 Simulating from the probability density function $f(x)$, which is non-zero over the finite range $[\theta, \alpha]$. The method used generates points (denoted by \circ and \times) uniformly at random over the rectangle shown. Points denoted by \circ are rejected (cf. Fig. 4.2), while the abscissae of the points \times are accepted as realizations of the random variable with probability density function $f(x)$. For illustration we have used the $B_c(3, 2.5)$ distribution, for which $\theta = 0$, $\alpha = 1$, $\delta = 0.3435$.

As the area of the rectangle in Fig. 5.4 is $\delta(\alpha - \theta)$, and the area under the curve is unity, we see that the probability of accepting a point is $1/(\delta(\alpha - \theta))$, and so the smaller δ is, the larger is the probability of acceptance and, correspondingly, the more efficient the method. This is, of course, why a larger value of δ was not used in Fig. 5.4.

There are two snags with the above approach. A rectangle is, as we have seen, a convenient shape within which to simulate a random uniform spread of points, but it clearly cannot be used if the density $f(x)$ has an infinite range, as we can only simulate uniform random variables over a finite range. Furthermore, the probability of rejection could become quite large: if the density of Fig. 5.4 was replaced by a spiked density, for instance, such as would result from a Laplace distribution, truncated to have a finite range. In such a case the simplicity gained from distributing points uniformly over a rectangular region could be more than offset by the cost of frequent rejection.

Both of these snags can be overcome by using as the enveloping curve a suitable multiple of a different probability density function from $f(x)$, as we shall now see. Consider a p.d.f. $h(x)$, with the same range as $f(x)$, but from which it is relatively easy to simulate. It is then simple to obtain a uniform scatter of points under $h(x)$, by taking points (X, Y) such that X has density $h(x)$, while the conditional density of Y given $X = x$ is $U(0; h(x))$. For a uniform scatter of points, the conditional p.d.f. of Y clearly must be of this form, while the X co-ordinate must have the property that for any pair (α, β) , with $\alpha < \beta$, $\Pr(\alpha \leq X < \beta) \sim \int_{\alpha}^{\beta} h(x) dx$, i.e. X must have probability density function $h(x)$.

If it were possible to choose $h(x)$ to be of a roughly similar shape to $f(x)$ and then to envelop $f(x)$ by $h(x)$, we would obtain the desired scatter of points under $f(x)$ by first obtaining a scatter of points under $h(x)$ and then rejecting just those which were under $h(x)$ but not under $f(x)$. While it is often possible to choose an appropriate $h(x)$ to be of similar shape to $f(x)$, it is clearly not possible to envelop $f(x)$ by $h(x)$, so that, for all x , $f(x) \leq h(x)$, since both $f(x)$ and $h(x)$ are density functions, and so $\int_{-\infty}^{\infty} f(x) dx = \int_{-\infty}^{\infty} h(x) dx = 1$. However, the solution to this last obstacle is easily obtained by, effectively, plotting $h(x)$ and the scatter of points obtained under $h(x)$ on stretchable paper, and then uniformly stretching the paper in a direction at right angles to the x -axis until $h(x) \geq f(x)$ for all x . Such stretching clearly does not change the uniformity of the scatter of the points. Mathematically this stretching is done, very simply, by taking as the conditional density of Y given $X = x$, $U(0, kh(x))$, where $k > 1$ is the stretching factor, and where X has probability density function $h(x)$.

Thus for suitable $h(x)$ and k , we have the following algorithm: if we write $g(x) = kh(x)$,

- (i) simulate $X = x$ from probability density function $h(x)$;
- (ii) simulate Y to be $Ug(x)$, where U is an independent $U(0, 1)$ random variable;

- (iii) accept $X = x$ as a realization of a random variable with probability density function $f(x)$ if and only if $Y < f(x)$.

The situation is illustrated in Fig. 5.5.

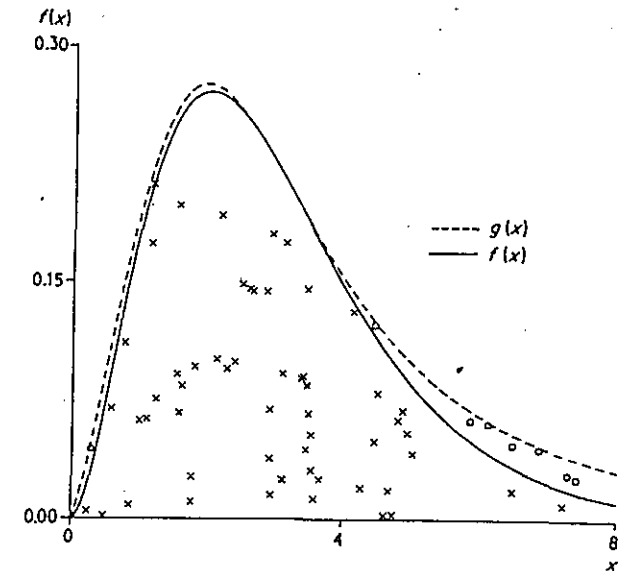


Figure 5.5 The points \times and \circ are uniformly and randomly distributed under the curve $g(x) = kh(x)$, where $k > 1$ is a constant, and $h(x)$ is a density from which it is easy to simulate. The points \circ lie above the density function $f(x)$ and so are rejected. The points \times are accepted and their abscissae are realizations of a random variable with probability density function $f(x)$. See Exercise 5.22 for an explanation of the p.d.f.'s used.

At first sight this algorithm seems unusual and confusing, since the test in (iii) concerns Y , but if the test is satisfied then it is $X = x$ which is accepted. However, in the light of the above discussion, we can now see that (iii) is just a component of testing whether a point constructed randomly and uniformly under $g(x)$ is also under $f(x)$.

The probability of rejection here is

$$\frac{\int_{-\infty}^{\infty} (g(x) - f(x)) dx}{\int_{-\infty}^{\infty} g(x) dx} = 1 - \frac{1}{k}$$

reflecting the importance of small k , subject to $k > 1$:

We choose $h(x)$ with shape and convenience in mind. The next two examples

provide two approaches for selecting k . The first example uses an exponential envelope to simulate normal random variables. An exponential envelope can only envelop half of the standard normal density, but it can envelop the 'half-normal' density, given by

$$f(x) = \sqrt{\left(\frac{2}{\pi}\right)} e^{-x^2/2} \quad \text{for } x \geq 0$$

i.e. $f(x) = 2\phi(x)$, for $x \geq 0$. If X has density function $f(x)$, then the random variable

$$\tilde{X} = \begin{cases} X & \text{with probability } \frac{1}{2} \\ -X & \text{with probability } \frac{1}{2} \end{cases}$$

clearly has the standard normal density $\phi(x)$ for $-\infty \leq x < \infty$. We shall therefore simulate from $\phi(x)$ by first simulating from $f(x)$, and then applying the above transformation, from \tilde{X} to X .

EXAMPLE 5.5 A rejection method for $N(0, 1)$ variables

Here

$$f(x) = \sqrt{\left(\frac{2}{\pi}\right)} e^{-x^2/2} \quad \text{for } x \geq 0$$

and

$$g(x) = ke^{-x} \quad \text{for } x \geq 0$$

One way of choosing k is to consider the condition for equal roots arising from setting

$$ke^{-x} = \sqrt{\left(\frac{2}{\pi}\right)} e^{-x^2/2}$$

as the roots in x of this equation correspond to the intersection of $g(x)$ and $f(x)$. If this equation has no real roots, then k is too large. If the equation has two distinct roots, then k is too small. The case of two equal roots corresponds to the smallest possible value of k , and the two curves touch, as shown in Fig. 5.6.

Setting $k \sqrt{\left(\frac{\pi}{2}\right)} = e^{x-x^2/2}$

results in a quadratic equation in x :

$$x^2 - 2x + 2 \log_e \left(k \sqrt{\left(\frac{\pi}{2}\right)} \right) = 0$$

which has equal roots if and only if

$$1 = 2 \log_e \left(k \sqrt{\left(\frac{\pi}{2}\right)} \right)$$

i.e. $k^2 \frac{\pi}{2} = e$

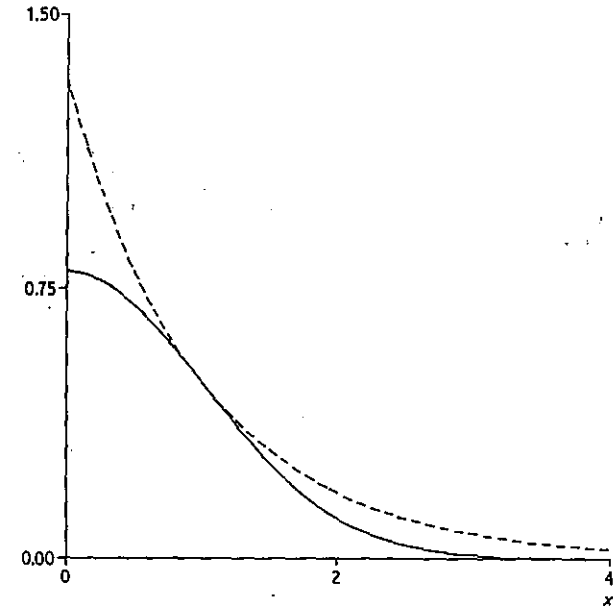


Figure 5.6 An illustration of the optimum choice of k . Here we illustrate the use of the exponential e^{-x} probability density function as the basis of an envelope for the half-normal density (solid line). The enveloping function is given by $\sqrt{\left(\frac{2e}{\pi}\right)} e^{-x}$ (dashed line), illustrated for $x \leq 4$, as is $f(x)$.

i.e. $k = + \sqrt{\left(\frac{2e}{\pi}\right)} \approx 1.3154892$

the equal roots occurring at $x = 1$, which is, in fact, also the point of inflexion for the half-normal density.

The algorithm therefore proceeds as follows:

- (a) Simulate X from density function, e^{-x} for $x \geq 0$. We know, from Equation (5.5) above, that we can do this by setting $X = -\log_e U_1$, where U_1 is a $U(0, 1)$ random variable. An alternative approach is given in Exercises 5.33-5.35.
- (b) If U_2 is an independent $U(0, 1)$ random variable, set $Y = kU_2e^{-X}$, i.e. $Y = kU_2U_1$.
- (c) Accept X if and only if,

$$Y < \sqrt{\left(\frac{2}{\pi}\right)} e^{-x^2/2}$$

i.e. $kU_1U_2 < \sqrt{\left(\frac{2}{\pi}\right)} e^{-x^2/2}$

i.e.
$$U_1 U_2 < \exp(-(1 + X^2)/2),$$

since
$$k = \sqrt{\left(\frac{2e}{\pi}\right)}.$$

Thus ultimately the algorithm does not involve k directly.

Finally, of course, we must convert the half-normal random variable X to the standard normal random variable \bar{X} . While this last stage can always be done by selecting a new $U(0, 1)$ random variable, and then testing whether it is greater or less than $\frac{1}{2}$, we note that as Y is $U(0, g(X))$, then conditional on

$$Y < \sqrt{\left(\frac{2}{\pi}\right)} e^{-x^2/2},$$

$$Y \text{ has a } U\left(0, \sqrt{\left(\frac{2}{\pi}\right)} e^{-x^2/2}\right) \text{ distribution,}$$

and the sign of \bar{X} can be decided by considering whether or not

$$Y < \frac{e^{-x^2/2}}{\sqrt{2\pi}}.$$

This is the same idea that was exploited in Exercise 4.2 and Section 4.4.1.

A BASIC program for this algorithm is shown in Fig. 5.7.

The reason for using e^{-x} as the p.d.f. for the basis of the envelope here, rather than any other $\lambda e^{-\lambda x}$ p.d.f. can be found from a consideration of the probability of rejection, $1 - 1/k$, and we see in Exercise 5.21 that $\lambda = 1$ minimizes this rejection probability.

```

10 RANDOMIZE
20 INPUT M
30 REM PROGRAM TO SIMULATE M STANDARD NORMAL
40 REM RANDOM VARIABLES, USING A REJECTION METHOD
50 REM WITH A HALF-NORMAL PDF ENVELOPED BY A
60 REM MULTIPLE OF THE EXPONENTIAL PDF WITH
70 REM PARAMETER 1
80 FOR I = 1 TO M
90 LET U1 = RND
100 LET U2 = RND
110 LET X = -LOG(U1)
120 LET B = .5*EXP(-.5*X*X/2)
130 LET C = U1*U2
140 IF C < B THEN 170
150 IF C < 2*B THEN 190
160 GOTO 90
170 PRINT -X
180 GOTO 200
190 PRINT X
200 NEXT I
210 END

```

Figure 5.7 BASIC program for the rejection method illustrated in Fig. 5.6.

The exponential function provides a suitable envelope for the half-normal probability density function, as the rate at which e^{-x} tends to zero as $x \rightarrow \infty$ is less than the rate at which $e^{-x^2/2}$ tends to zero as $x \rightarrow \infty$.

A general way of finding k is to note that we want k to satisfy $kh(x) \geq f(x)$ for all x , and that we cannot have equality here for all x . k is therefore given by

$$k = \max_x \left(\frac{f(x)}{h(x)} \right)$$

if a finite maximum can be found, as then $kh(x) \geq f(x)$ for all x , with equality for at least one x .

A finite maximum will not result if $h(x)$ is unsuitable as a basis for an envelope of $f(x)$. For instance, we could have $h(x) = 0$ when $f(x) > 0$, or we might try setting $f(x) = e^{-x}$ and $h(x) = e^{-x^2/2}$. In this latter case,

$$\log(f(x)/h(x)) = \frac{x^2}{2} - x$$

which increases without bound as $x \rightarrow \infty$.

This approach should work, however, if a suitable $h(x)$ has been found. In this example we have

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

$$y = \log(f(x)/h(x)) = \log\left(\sqrt{\left(\frac{2}{\pi}\right)}\right) + x - \frac{x^2}{2}$$

$$\frac{dy}{dx} = 1 - x$$

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

Thus we maximize $f(x)/h(x)$ by setting $x = 1$, to give, as before, $k = \sqrt{\left(\frac{2e}{\pi}\right)}$.

In Section 4.3 we have already seen one way of simulating $\Gamma(n, \lambda)$ random variables, when n is a positive integer. The next example provides an alternative approach, for the case $n > 1$, using rejection, and an exponential envelope as in the last example. This approach may also be used when $n > 1$ is not integral.

Here we take $\lambda = 1$ for simplicity. If a random variable X results, then the new random variable $Y = X/\lambda$ will have a $\Gamma(n, \lambda)$ distribution, from the theory of Section 2.12 (see Exercise 2.2).

*EXAMPLE 5.6 A rejection method for $\Gamma(n, 1)$ variables.

Here
$$f(x) = \frac{x^{n-1} e^{-x}}{\Gamma(n)} \quad \text{for } x \geq 0, \text{ and } n > 1$$

$$g(x) = ke^{-x/n}/n \quad \text{for } x \geq 0.$$

As $n > 1$, then as $x \rightarrow \infty$, $f(x) \rightarrow 0$ faster than $g(x)$, implying that $g(x)$ is a suitable enveloping function for $f(x)$.

Let $y = f(x)/g(x)$. We seek k by maximizing y with respect to x .

$$\log_e y = (n-1)\log_e x - x + \frac{x}{n} + \log_e(n/\Gamma(n))$$

$$\frac{d}{dx}(\log_e y) = \frac{n-1}{x} - 1 + \frac{1}{n}$$

$$\frac{d^2}{dx^2}(\log_e y) = \frac{1-n}{x^2}$$

Thus, as $n > 1$, we maximize y when

$$\frac{n-1}{x} = 1 - \frac{1}{n}$$

i.e. when $x = n$, and so

$$k = n^n e^{1-n} / \Gamma(n)$$

It is now a simple matter to derive the following algorithm. Let U be a $U(0, 1)$ random variable, and let E be an independent exponential random variable with parameter n^{-1} . If

$$t(x) = \left(\frac{x}{n}\right)^{n-1} \exp\left[(1-n)\left(\frac{x}{n} - 1\right)\right] \quad \text{for } x \geq 0$$

then conditional on $t(E) \geq U$, E has the required gamma p.d.f.

The above method, due originally to G. S. Fishman, is described by Atkinson and Pearce (1976). Of course, any density function $f(x)$ can be enveloped by a wide variety of alternative functions, and an alternative rejection method for simulating gamma random variables is given in Exercise 5.22.

For distributions over a finite range, an alternative approach is to envelop the distribution with a suitable polygon and then use the method of Hsuan (1979). A generalization of the rejection method is given in Exercise 5.29.

5.4 The composition method

Here again we encounter a general method suitable for discrete and continuous random variables. We shall begin our discussion of this method with an illustration from Abramowitz and Stegun (1965, p. 951).

For a binomial $B(5, 0.2)$ distribution we have the following probabilities, given to four places of decimals:

i	p_i
0	0.3277
1	0.4096
2	0.2048
3	0.0512
4	0.0064
5	0.0003

If we take p_0 as an example, we can write

$$p_0 = 0.3277 = 0.9 \times \frac{3}{9} + 0.07 \times \frac{2}{7} + 0.027 \times \frac{7}{27} + 0.003 \times \frac{7}{30}$$

and similarly,

$$p_1 = 0.4096 = 0.9 \times \frac{4}{9} + 0.07 \times \frac{0}{7} + 0.027 \times \frac{9}{27} + 0.003 \times \frac{6}{30}$$

$$p_2 = 0.2048 = 0.9 \times \frac{2}{9} + 0.07 \times \frac{0}{7} + 0.027 \times \frac{4}{27} + 0.003 \times \frac{8}{30}$$

and so on, so that in general,

$$p_i = 0.9 r_{i1} + 0.07 r_{i2} + 0.027 r_{i3} + 0.003 r_{i4} \quad \text{for } 0 \leq i \leq 5 \quad (5.6)$$

where $\{r_{i1}\}$, $\{r_{i2}\}$, $\{r_{i3}\}$ and $\{r_{i4}\}$ are all probability distributions over the same range, $0 \leq i \leq 5$.

We can see that in (5.6),

$$0.9 = 10^{-1} \times (\text{sum of digits in first decimal place of the } p_i)$$

$$0.07 = 10^{-2} \times (\text{sum of digits in second decimal place of the } p_i)$$

and so on

while, for example,

$$r_{01} = \frac{0.3}{0.9} = \frac{3}{9}$$

$$r_{11} = \frac{0.4}{0.9} = \frac{4}{9}$$

$$r_{21} = \frac{0.2}{0.9} = \frac{2}{9}$$

$$r_{02} = \frac{0.02}{0.07} = \frac{2}{7}$$

etc.

This explains the derivation of (5.6). We can now use (5.6) to simulate from the $\{p_i\}$ distribution as follows:

(i) Simulate a discrete random variable, R , say, according to the distribution:

j	$\Pr(R = j)$
1	0.9
2	0.07
3	0.027
4	0.003

(ii) If $R = j$, simulate from the $\{r_{ij}\}$ distribution for $1 \leq j \leq 4$. If the resulting random variable is denoted by X ,

$$\Pr(X = i) = \sum_{j=1}^4 \Pr(R = j)r_{ij} \quad (\text{see for example } ABC, \text{ p. 85})$$

i.e. $\Pr(X = i) = p_i$

i.e. X has the required binomial distribution.

Of course, a small amount of approximation has taken place here, as we have written the $\{p_i\}$ only to four places of decimals. Nevertheless, this approach may be used for any discrete distribution. While one has to simulate from two distributions $\{\Pr(R = j); 1 \leq j \leq 4\}$ and $\{r_{ij}\}$, most (97%) of the time one is simulating from $\{r_{i1}\}$ and $\{r_{i2}\}$, and these component discrete distributions are of a very simple form. A disadvantage of this method is the need to store the component distributions. In (5.6) we have written the $\{p_i\}$ distribution as a mixture, or composition, of the $\{r_{ij}\}$ distributions; a further example of this kind is to be found in Exercise 5.42. We shall now consider the analogous procedure for continuous random variables.

It is not unusual to encounter probability density functions which are

mixtures of other probability density functions, say

$$f(x) = \alpha f_1(x) + (1 - \alpha)f_2(x) \quad 0 < \alpha < 1 \quad (5.7)$$

In psychology, for example, bimodal histograms of reaction times are sometimes encountered, which may reflect a tendency for subjects to behave in some standard fashion a proportion α of the time, producing reaction times with probability density function $f_1(x)$, say, but the remainder of the time, possibly due to a loss in concentration, to produce reaction times that tend to be longer than before, with probability density function $f_2(x)$, say. Cox (1966) provides further discussion of this example.

Another example is provided by human height histograms, which could be bimodal due to a mixture of different male and female height-histograms. However, samples from such mixtures may not obviously reflect the mixture form of the underlying p.d.f., as is the case in the histogram of Fig. 5.8.

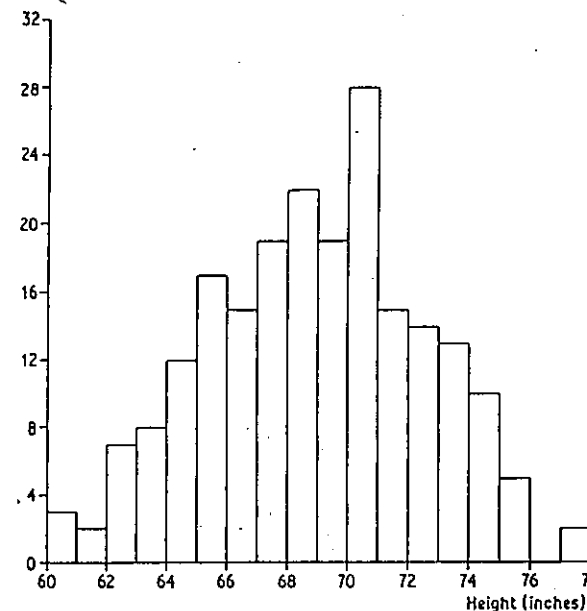


Figure 5.8 Histogram describing the heights of some undergraduates at the University of Kent (taken from Fuller and Lury, 1977, p. 14). For the 142 male undergraduates, heights range from 63 to 77 inches, with a modal height of 70 inches; for the 69 female undergraduates, heights range from 60 to 70 inches, with a modal height of 65 inches.

Indeed, we shall see that in many applications in simulation the mixture form of (5.7) is adopted solely for convenience, even for unimodal distributions such as the normal distribution. The convenience arises if α is fairly large and

$f_1(x)$ is a probability density function which is appreciably easier to simulate from than $f(x)$ itself. If we sample from $f_1(x)$ with probability α , and from $f_2(x)$ with probability $(1 - \alpha)$, then because of the relationship of (5.7) we obtain a random variable, X , with probability density function $f(x)$. We see this simply as follows:

$$\begin{aligned} \Pr(X \leq x) &= \alpha \Pr(X \leq x | \text{sample from } f_1(x)) + (1 - \alpha) \Pr(X \leq x | \text{sample from } f_2(x)) \\ &= \alpha \int_{-\infty}^x f_1(y) dy + (1 - \alpha) \int_{-\infty}^x f_2(y) dy \\ &= \int_{-\infty}^x f(y) dy \quad \text{by (5.7)} \end{aligned}$$

Let us now consider two examples which illustrate the use of the method.

EXAMPLE 5.7

Suppose we want to simulate random variables with the p.d.f. of Fig. 5.9.

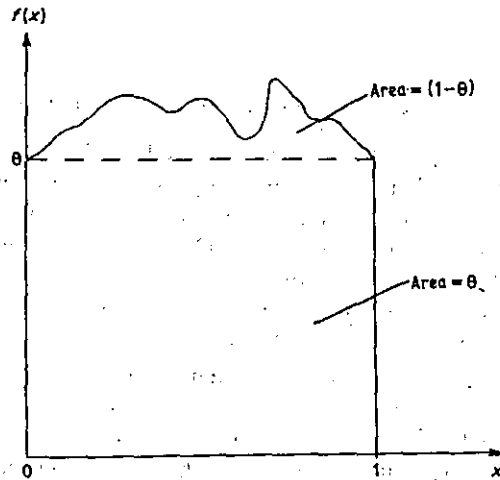


Figure 5.9 An unusual probability density function $f(x)$, from which we shall simulate using a composition, the first density, $f_1(x)$, of which is the $U(0, 1)$ density.

We note here that we can write

$$f(x) = \theta + f(x) - \theta \quad \text{for any } 0 \leq x \leq 1$$

i.e.,
$$f(x) = \theta \times 1 + (1 - \theta) \left(\frac{f(x) - \theta}{1 - \theta} \right) \quad (5.8)$$

As $\int_0^1 f(x) dx = 1$, then $\theta < 1$, and (5.8) is of the same form as (5.7). To simulate from $f(x)$, with probability θ we simply select a $U(0, 1)$ random variable, while with probability $(1 - \theta)$ we simulate from the p.d.f.,

$$f_2(x) = \left(\frac{f(x) - \theta}{1 - \theta} \right)$$

which has subsumed the features of $f(x)$ which made it a difficult p.d.f. from which to simulate. We can simulate from both $f(x)$ and $f_2(x)$ using a rejection method, but the advantage of the composition of (5.8) is that one only simulates from $f_2(x)$ with probability $(1 - \theta)$, and in the illustration of Fig. 5.9, $(1 - \theta)$ is appreciably less than 0.5.

EXAMPLE 5.8

A random variable X with the simple beta probability density function

$$f(x) = 6x(1 - x) \quad \text{for } 0 \leq x \leq 1$$

can be simulated quite easily by either the table-look-up method, or the rejection method (see Exercise 5.18). Figure 5.10 shows how we may use a

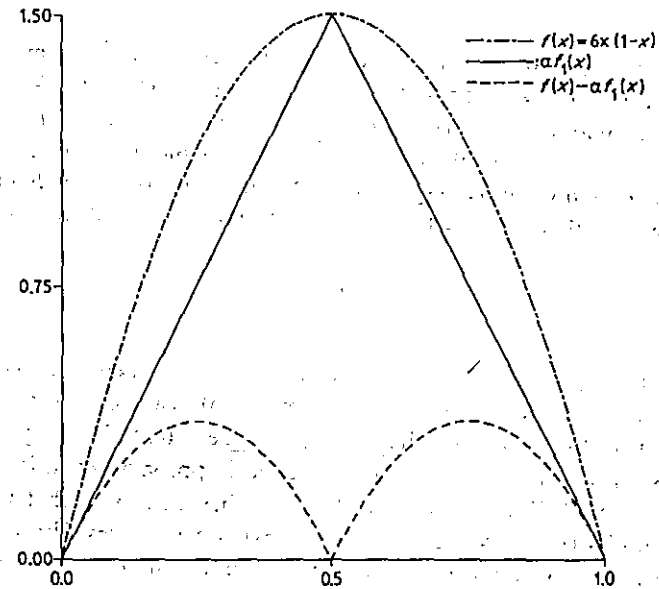


Figure 5.10 The beta density function, $f(x) = 6x(1 - x)$ and the basis for a composition.

composition method. Here, $f_1(x)$ is simply the symmetric triangular density over $(0,1)$, i.e.

$$f_1(x) = \begin{cases} 4x & \text{for } 0 \leq x \leq 0.5 \\ 4(1-x) & \text{for } 0.5 \leq x \leq 1 \end{cases}$$

From simple geometrical consideration we see that we must have $\alpha \leq \frac{3}{4}$, and as we want α to be as large as possible, we take $\alpha = \frac{3}{4}$. The second density in the composition is then given by

$$f_2(x) = \frac{f(x) - \alpha f_1(x)}{1 - \alpha} = \begin{cases} 12x(1-2x) & \text{for } 0 \leq x \leq 0.5 \\ 12(1-2x)(x-1) & \text{for } 0.5 \leq x \leq 1 \end{cases}$$

We shall leave the reader to consider how we might simulate from $f_2(x)$.

In general, suppose we have a probability density function $f(x)$, and that $f_1(x)$ is a probability density function of roughly similar shape, but that it is appreciably easier to simulate from $f_1(x)$ than from $f(x)$. We shall see shortly why we want $f(x)$ and $f_1(x)$ to be of similar shape.

We can formally write, for any α in the range $0 < \alpha < 1$,

$$f(x) = \alpha f_1(x) + (1 - \alpha) \left(\frac{f(x) - \alpha f_1(x)}{1 - \alpha} \right)$$

and from the above discussion we see that we can simulate from $f(x)$ by simulating from $f_1(x)$ with probability α , and from $f_2(x) = (f(x) - \alpha f_1(x)) / (1 - \alpha)$ with probability $(1 - \alpha)$. As $f_1(x)$ is chosen to be relatively easy to simulate from, we clearly want α to be as large as possible. The constraint on α is that for all x we must have $f(x) - \alpha f_1(x) \geq 0$, in order to ensure that $f_2(x)$ is also a probability density function (it is easy to see that its integral is unity). Now if

$$\alpha = \min_x \left(\frac{f(x)}{f_1(x)} \right)$$

and a positive, non-zero minimum can be found, then $\alpha \leq f(x)/f_1(x)$, i.e. $f(x) - \alpha f_1(x) \geq 0$, as required, and there is at least one x for which $\alpha f_1(x) = f(x)$, so that a larger value of α cannot be found. This approach to finding α is, of course, analogous to the general approach given in the last section for finding k . Here we can consider α as shrinking $f_1(x)$ so that it just fits completely under $f(x)$, as we have seen in the last two examples. This of course explains why we seek an $f_1(x)$ to be of roughly similar shape to $f(x)$: the more similar in shape $f(x)$ and $f_1(x)$ are, then the larger the shrinking parameter α can be. For rejection, then, we envelop $f(x)$, but for composition it is $f(x)$ itself that plays the enveloping rôle. The method generalizes in a straightforward way, so

that we could repeat the procedure for $f_2(x)$, and so on, ending ultimately with the mixture:

$$f(x) = \sum_{i=1}^{n+1} \alpha_i f_i(x)$$

in which

$$\sum_{i=1}^{n+1} \alpha_i = 1$$

and

$$\alpha_i > 0 \quad \text{for } 1 \leq i \leq n+1,$$

all the $f_i(x)$ are probability density functions, and

$$f_{n+1}(x) = \left(f(x) - \sum_{i=1}^n \alpha_i f_i(x) \right) / \left(1 - \sum_{i=1}^n \alpha_i \right)$$

In choosing n , one has to counterbalance the difficulty of simulating from the final density function, $f_{n+1}(x)$, with the size of α_{n+1} , and the general desirability of keeping n small.

In the last two examples, all the p.d.f.'s considered had a finite range. As we shall see in the next section, it sometimes happens that $f(x)$ has an infinite range, but $f_1(x)$ has a finite range. In such a case, we have a range of x for which $f_1(x) = 0$, but $f_2(x) > 0$. In fact, as is shown in the next section, we can also have $f_2(x) = 0$ and $f_1(x) > 0$ for certain x .

*5.5 Combining methods for simulating normal random variables

In recent years much ingenuity has been devoted to devising composition methods for the standard normal probability density function. These approaches have also employed rejection, table-look-up and particular methods, and it is fascinating to see all of these different tools put to work on the one problem. As with the rejection method, many different compositions can be formed for any one probability density function, and here we shall just consider one, for the $N(0, 1)$ density. Due to Marsaglia and Bray (1964), the method gives rise to what has been termed their 'convenient' algorithm. Other methods are discussed in Exercises 5.36-5.38.

What many of the different methods proposed for the $N(0, 1)$ p.d.f. have in common, however, is the initial isolation of the tails of the normal density function, and the first composition usually taken is:

$$\frac{e^{-x^2/2}}{\sqrt{2\pi}} = \alpha \phi_1(x) + (1 - \alpha) \phi_2(x) \tag{5.9}$$

in which

$$\phi_1(x) = \begin{cases} \frac{1}{\alpha} \frac{e^{-x^2/2}}{\sqrt{2\pi}} & \text{for } -3 \leq x \leq 3 \\ 0 & \text{for } |x| > 3 \end{cases}$$

and

$$\phi_2(x) = \begin{cases} \frac{1}{(1-\alpha)\sqrt{2\pi}} \frac{e^{-x^2/2}}{\sqrt{2\pi}} & \text{for } |x| > 3 \\ 0 & \text{for } -3 \leq x \leq 3 \end{cases}$$

where

$$1-\alpha = 2 \int_{-\infty}^{-3} \frac{e^{-x^2/2}}{\sqrt{2\pi}} \approx 0.0027$$

to 4 places of decimals. Here, then, is an instance of the two component p.d.f.'s in (5.7) having different ranges. $|x| > 3$ is used to define the normal p.d.f. tails as 3 is suitably large and, as we shall see, ties in conveniently with the approaches adopted in what follows.

The composition of (5.9) means that most of the time we simulate from the expanded normal density, $\phi_1(x)$, over the finite range $|x| \leq 3$, while with the very small probability $(1-\alpha)$ we simulate from the p.d.f. $\phi_2(x)$, formed by expanding the tail areas from the standard normal p.d.f.

Let us consider $\phi_2(x)$ first of all. A random variable X with probability density function $\phi_2(x)$ is simply an $N(0, 1)$ random variable, conditioned to be $|X| \geq 3$. Such random variables result from the Box-Muller or Polar Marsaglia methods of Section 4.2 as follows: in the Box-Muller notation of Equation (4.1), if the exponential variable $-2 \log_e U_1 > 9$, then from the geometrical explanation of Section 4.2.1, there is a good chance that at least one of N_1 and N_2 is greater than 3 in modulus, as required. Certainly, if $-2 \log_e U_1 < 9$ then neither of N_1 and N_2 will be greater than 3, and so the standard approach of Section 4.2 towards constructing the conditioned normal variables that we require would be very wasteful. However, as is discussed in Exercise 5.24, $Y = 9 - 2 \log_e U_1$ is a random variable with the required exponential distribution, but conditional on being greater than 9. We can therefore simulate from the p.d.f. $\phi_2(x)$ by replacing $-2 \log_e U_1$ in Equation (4.1) by $(9 - 2 \log_e U_1)$, but only accepting a resulting N_1 or N_2 value if it is greater than 3 in modulus. Correspondingly, we can modify the Polar Marsaglia method by replacing $(-2 \log_e W)$ in Equation (4.2) by $(9 - 2 \log_e W)$, and proceeding in the same fashion.

There is more discussion of tail area simulation in the solution to Exercise 5.38. So far we have used the particular approaches of Section 4.2, and the table-look-up method to give exponential random variables of mean 2. Now we shall return to $\phi_1(x)$.

Figure 5.11 illustrates $\phi_1(x)$ and also the probability density function of the random variable

$$Y = 2(U_1 + U_2 + U_3 - 1.5) \quad -3 \leq Y \leq 3$$

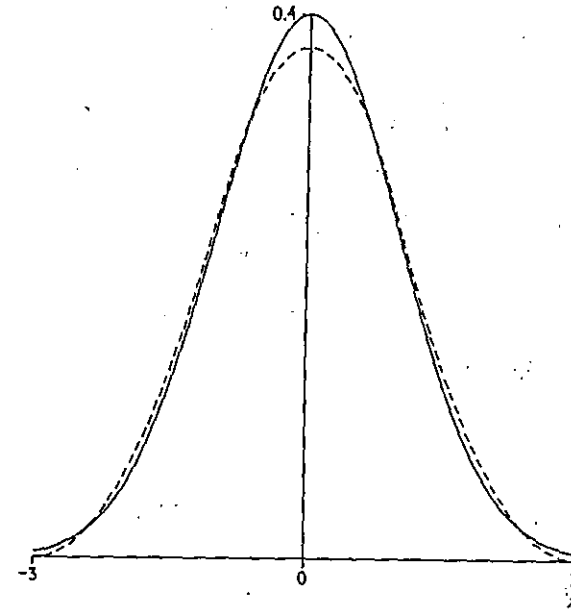


Figure 5.11 The preliminary to a composition method. Here we want to simulate from $\phi_1(x)$ (denoted by a solid line) the standard normal p.d.f. conditioned to the range $|x| \leq 3$. It is proposed to use as the first p.d.f. in the composition, $f_1(x)$ (dashed line), the density of $Y = 2(U_1 + U_2 + U_3 - 1.5)$, where U_1, U_2 and U_3 are independent $U(0, 1)$ random variables.

in which U_1, U_2 and U_3 are independent $U(0, 1)$ random variables. (See Exercise 4.8). The two curves are of similar shape, and Y is clearly easy to simulate: We shall now, therefore, seek a composition for $\phi_1(x)$, with the first p.d.f. in the composition being $f_1(x)$, the probability density function of Y , given by (see Exercise 4.8)

$$f_1(x) = \begin{cases} (3-x^2)/8 & -1 \leq x \leq 1 \\ (3-|x|)^2/16 & 1 \leq |x| \leq 3 \\ 0 & |x| \leq 3 \end{cases}$$

Using the approach outlined in the last section, we want to minimize $q(x) = \phi_1(x)/f_1(x)$ with respect to x varying over the range $|x| \leq 3$. Because $f_1(x)$ is specified differently over different ranges for x , we shall deal with these different ranges separately.

First let us consider $0 \leq x \leq 1$. Here,

$$q(x) = \frac{8 e^{-x^2/2}}{\alpha(3-x^2)\sqrt{2\pi}}$$

$$l(x) = \log q(x) = \text{constant} - \frac{x^2}{2} - \log(3 - x^2)$$

$$\frac{d}{dx} l(x) = -x + \frac{2x}{(3 - x^2)}$$

= 0 when $x = 0$ and when $3 - x^2 = 2$, i.e. $x = 1$

$$\frac{d^2 l(x)}{dx^2} = -1 + \frac{2}{(3 - x^2)} + \frac{4x^2}{(3 - x^2)^2}$$

i.e. $\frac{d^2 l(x)}{dx^2}$ is negative when $x = 0$, and positive when $x = 1$.

Next we shall consider the range $1 \leq x \leq 3$.

Here,
$$q(x) = \frac{16e^{-x^2/2}}{\alpha(3 - x)^2 \sqrt{2\pi}}$$

$$l(x) = \log q(x) = \text{constant} - \frac{x^2}{2} - 2 \log(3 - x)$$

$$\frac{d}{dx} l(x) = -x + \frac{2}{(3 - x)}$$

= 0 when $3x - x^2 = 2$

i.e. when $x = 1$ and when $x = 2$.

$$\frac{d^2}{dx^2} l(x) = -1 + \frac{2}{(3 - x)^2}$$

i.e. $d^2 l(x)/dx^2$ is negative when $x = 1$, and positive when $x = 2$, revealing a minimum to $q(x)$ when $x = 2$.

Thus for the case of $x \geq 0$, $q(x)$ has a maximum when $x = 0$, a saddle-point when $x = 1$, and a minimum when $x = 2$. We need not consider the case $x \leq 0$ separately because of the symmetry present, and so we can conclude that $q(x)$ has minima at $x = \pm 2$ in the range $|x| \leq 3$.

Hence if we write

$$\phi_1(x) = \alpha_1 f_1(x) + \alpha_2 f_2(x)$$

$$\alpha_1 = \frac{\phi_1(2)}{f_1(2)} = \frac{16e^{-2}}{\alpha \sqrt{2\pi}}$$

and overall, from considering the compositions for $e^{-x^2/2}/\sqrt{2\pi}$ and $\phi_1(x)$, we simulate from $f_1(x)$ with probability

$$\alpha\alpha_1 = \frac{16e^{-2}}{\sqrt{2\pi}} \approx 0.8638$$

Here we see a dramatic demonstration of the possible power of the composition method: over 86 per cent of the time we can expect to simulate an

$N(0, 1)$ random variable by simply taking a linear function of the sum of three independent $U(0, 1)$ random variables.

In fact there is still more of interest remaining in this example. With probability $\alpha\alpha_2$ we must simulate from the probability density function

$$f_2(x) = \left(\frac{\phi_1(x) - \alpha_1 f_1(x)}{1 - \alpha_1} \right) \quad -3 \leq x \leq 3$$

i.e. with probability $\alpha\alpha_2 = \alpha(1 - \alpha_1) = (0.9973 - 0.8638) = 0.1335$.

Figure 5.12 presents a graph of $\phi_1(x) - \alpha_1 f_1(x)$, and the form of the graph suggests proceeding further with the composition for $\phi_1(x)$, by now using a triangular p.d.f. and setting

$$f_2(x) = \beta g(x) + (1 - \beta)h(x)$$

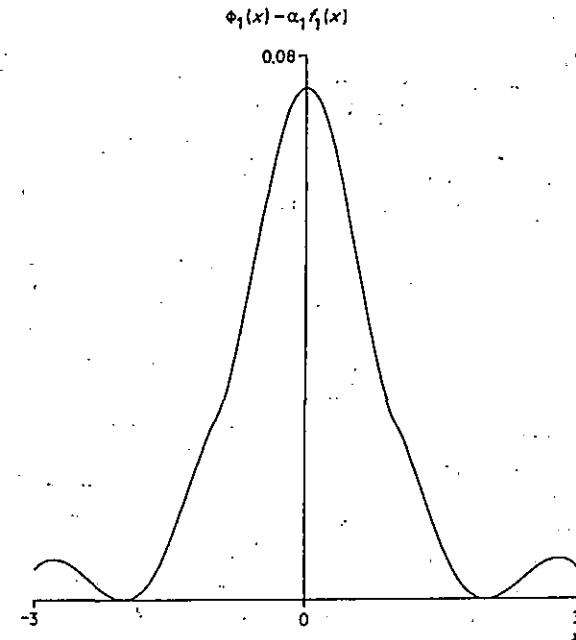


Figure 5.12 The residual curve $\phi_1(x) - \alpha_1 f_1(x)$ following the composition method envisaged in Fig. 5.11.

where
$$g(x) = \begin{cases} (6 - 4|x|)/9 & \text{for } |x| \leq 1.5 \\ 0 & \text{for } |x| > 1.5 \end{cases}$$

$g(x)$ is simply the probability density function of

$$Y = 1.5(U_1 + U_2 - 1)$$

where U_1 and U_2 are independent $U(0, 1)$ random variables (see Exercise 4.8). In this case, with the aim of determining β , $f_2(x)/g(x)$ cannot be minimized explicitly, but a numerical method such as Newton-Raphson readily provides us with $\beta \approx 0.8292$, the minimum occurring at $x = \pm 0.8739$. We thus simulate from $g(x)$ with probability $\alpha(1 - \alpha)\beta = 0.1107$, so that over 97 per cent of the time we use the two simple p.d.f.'s $f_1(x)$ and $g(x)$.

The three compositions that we have dealt with here can be written as one, to give

$$\frac{e^{-x^2/2}}{\sqrt{2\pi}} = 0.8638 f_1(x) + 0.1107 g(x) + 0.0027 t(x) + 0.0228 r(x) \quad (5.10)$$

for $-\infty \leq x \leq \infty$

where $t(x)$ is the tail-area p.d.f. which we considered earlier, and $r(x)$ is the p.d.f. that remains for $|x| \leq 3$.

We simulate from the p.d.f. $r(x)$ only with probability 0.0228, and as $r(x)$ is of a fairly complicated form (shown in Fig. 5.18) we can simulate from it by means of simple rejection, using a rectangular enveloping region over the finite range $|x| \leq 3$, with, it can be shown, probability 0.53 of rejection (see Exercises 5.16 and 5.39).

The above derivation of (5.10) should not disguise the fact that (5.10) is a description of one way of dividing up the area under the $N(0, 1)$ probability density function, precisely as was done in a different case in Example 5.7. The end-result is shown in Fig. 5.13.

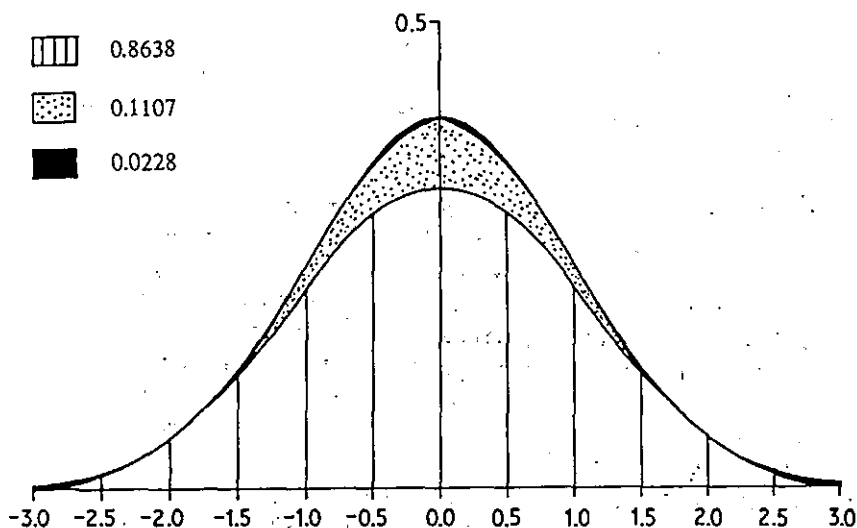


Figure 5.13 A representation of the composition given in Equation (5.10) for the range $|x| \leq 3$. The regions shown have the areas indicated above.

5.6 Discussion and further reading

The examples considered in this chapter form only a very small subset of the many interesting and complicated approaches that have been devised in recent years. For instance, having obtained a normal random variable, then one can even use the normal distribution itself as an enveloping distribution; see, for example, Ahrens and Dieter (1974) and Atkinson (1979). More examples are to be found in the exercises.

We have seen that uniform $U(0, 1)$ random variables are the building-blocks for the simulation of any other random variable. Complicated algorithms utilizing composition and rejection methods, and sometimes requiring the storage of a large number of constants, are designed for use on computers that work to high precision. These algorithms are often programmed in machine code and tend to be the most efficient. They are therefore most suitable if one is seeking to provide a computer with an efficient package of programs for simulating a variety of random numbers, which will be used frequently by a large number of individuals. Comparisons of different algorithms, using speed and efficiency, have been undertaken by a number of authors—see, for example, Atkinson and Pearce (1976), Kinderman and Ramage (1976) and Ripley (1983b). Appleton (1976) pointed out that certain methods can be programmed in the programming language APL, to take advantage of APL's vector-handling capabilities, and as an example he found the Box-Muller method to be 30 times faster than the Marsaglia and Bray 'convenient' method, when both were programmed in APL. This is partly due to the fact that APL programs are interpreted, rather than compiled, as are FORTRAN programs. Using FORTRAN, Atkinson and Pearce (1976) found Box-Muller to be roughly twice as slow as the convenient method. Distributed array processing is another factor which could influence the comparison of different algorithms (cf. Exercise 3.16).

Ripley (1983b) provides a list of relatively efficient simple algorithms for a variety of distributions. Most users of main-frame computers will be likely to use library subroutines such as those described in Section A1.1. Because of the time-lag before library subroutines are changed to accommodate new developments, these programs may not always be the most efficient. Each individual clearly has to experiment with the facilities available if it is suspected that long generation times of random variables could render a simulation impractical.

Of course, the simplest way for human beings to simulate random variables is to use tables of realizations of such random variables, such as those by Wold (1954), providing normal random variables, and those by Barnett (1965), which provide exponential random variables. In the absence of such tables, the table-look-up approach is also easily performed by hand if one has suitable tables of cumulative distribution functions, and only a small-scale simulation is

envisaged. Some such tables can be found in Harter (1964), Lieberman and Owen (1961), Mardia and Zemroch (1978), Neave (1978), Odeh, *et al.* (1977), Williamson and Bretherton (1963) and Worsdale (1975).

Simulation of discrete random variables by the table-look-up method can be very time consuming. This occurs with the Poisson distribution, for example, if it has large mean, in which case the particular method for this distribution, described in the last chapter, will also be inefficient. There is further discussion of this point in Exercises 5.3 and 5.4. The range-dividing technique, discussed in Section 5.1, can be generalized by dividing the range into $d > 2$ parts, as in Neave (1972), who provides ALGOL programs for several discrete distributions. A faster search procedure is the optimum binary tree search described in Knuth (1968, p. 400). As can be seen from Section A1.1, the NAG library of computer programs simulates all discrete distributions by first of all establishing a reference vector of cumulative sums, and then performing an indexed search by means of the routine GOSEYF. The IMSL routine for the table-look-up method for a general discrete distribution is GGDT (see Section A1.1).

The polar Marsaglia method of Section 4.2.2 shows that the ratio V_1/V_2 of the co-ordinates of a point uniformly distributed over a disc of unit radius and centred on the origin has a Cauchy distribution (see Exercise 5.8). Kinderman and Monahan (1977) have generalized this result to provide a new general method for simulating random variables, viz., the *ratio* method—see Ripley (1983b) for illustrations of its use. A further new general method is the *alias* method for discrete random variables, described in Exercise 5.42.

In this chapter we have only considered univariate random variables, but table-look-up, rejection and composition methods may also be used for multivariate random variables. Kemp and Loukas (1978a, b) consider the table-look-up method for a bivariate Poisson distribution, and the table-look-up method for bivariate Poisson and normal distributions is discussed in Exercises 5.10 and 5.11. Best and Fisher (1979) use a rejection method on the circle, enveloping the von Mises distribution with a wrapped Cauchy distribution.

We shall conclude this chapter with some further discussion of methods for simulating normal random variables.

*5.7. Additional approaches for normal random variables

The table-look-up method for normal random variables is difficult to program for computers because of the intractable form of the standard normal cumulative distribution function, $\Phi(x)$, and its inverse, $\Phi^{-1}(x)$. Various authors have approached this problem by providing approximate methods—see, for example, Zelen and Severo (1966) and Wetherill (1965). Wetherill's approach employs the attractive idea that an efficient algorithm can result

from using one approximation to $\Phi^{-1}(x)$ in the middle of the range for x , but another, more complicated algorithm in the tails, which would be used far less frequently. This idea is simply providing a composition method, the components of which are simulated using approximate table-look-up methods. Some other approaches are described below.

Because of the similar shapes of the normal and logistic probability density functions, it is natural to try to approximate the normal cumulative distribution function by the simple logistic cumulative distribution function. In order to obtain a good match over the middle of the range, the logistic cumulative distribution function that may be used is

$$F_1(x) = \left[1 + \exp\left(-2\sqrt{\left(\frac{2}{\pi}\right)x}\right) \right]^{-1} \quad -\infty \leq x \leq \infty$$

as this curve has the same slope at $x = 0$ as does $\Phi(x)$. An alternative possibility which might be considered is the logistic cumulative distribution function,

$$F_2(x) = \left[1 + \exp\left(-\frac{\pi x}{\sqrt{3}}\right) \right]^{-1} \quad -\infty \leq x \leq \infty$$

corresponding to a random variable with zero mean and unit variance. $F_1(x)$ and $F_2(x)$ are illustrated in Fig. 5.14, for $0 \leq x \leq 3$.

Table 5.1 is taken from Page (1977), who tries to improve a logistic approximation by adding an extra parameter, resulting in the cumulative distribution function

$$G(x) = \{1 + \exp[-2a_1x(1 + a_2x^2)]\}^{-1} \quad -\infty \leq x \leq \infty$$

Note that as the coefficient of the new parameter, a_2 , is x^3 , and not x^2 , which may have been considered a more natural choice, then we preserve the property $G(x) + G(-x) = 1$, and the corresponding probability density function is symmetric about $x = 0$.

If $a_1 = \sqrt{2/\pi}$, and a_2 is chosen by least squares, then a value of $a_2 = 0.044715$ is obtained. A slightly better approximation is obtained by allowing both a_1 and a_2 to be chosen by least squares, but the advantage of keeping $a_1 = \sqrt{2/\pi}$ is that if one wanted to approximate $\Phi(x)$ this way on a hand-calculator, only one constant needs to be remembered, most calculators having a ' π ' key. To simulate approximate $N(0, 1)$ random variables we need $\bar{x} = G^{-1}(U)$ (see Exercise 5.9). Some examples are given in Table 5.1.

Hamaker (1978) and Schmeiser (1979) provide further approximations that are suitable for computation on a hand-calculator, and more recent work is described in Bailey (1981) and Lew (1981).

Kinderman and Ramage (1976) use an even simpler p.d.f. for $f_1(x)$, the first p.d.f. in a composition for the standard normal density, than that resulting from the sum of three $U(0, 1)$ random variables. In their case, they used the p.d.f. of the sum of just two $U(0, 1)$ random variables, as illustrated in Fig. 5.15.

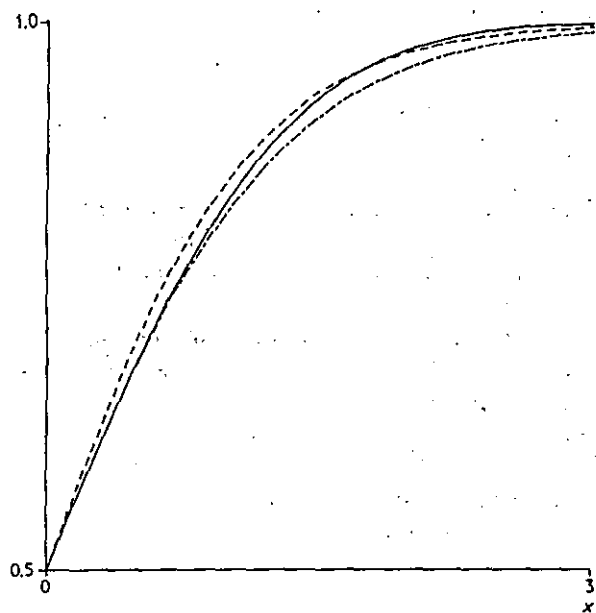


Figure 5.14 An illustration for $0 \leq x \leq 3$ of two logistic cumulative distribution functions, (---): $F_1(x) = \left[1 + \exp\left(-2\sqrt{\left(\frac{2}{\pi}\right)x}\right)\right]^{-1}$ and (-·-·-): $F_2(x) = \left[1 + \exp\left(-\frac{\pi x}{\sqrt{3}}\right)\right]^{-1}$, either of which may be used as a rough approximation to the normal cumulative distribution function, $\Phi(x)$, denoted by (—).

Table 5.1 Approximating the standard normal cumulative distribution function $\Phi(x)$. Two possible approximations are $F_1(x)$ and $G(x)$, explained in the text. \bar{x} results from inverting $G(x)$ (from Page, 1977).

x	$1 - \Phi(x)$	$1 - F_1(x)$	$1 - G(x)$	\bar{x}
0	0.5	0.5	0.5	0
0.1	0.460 172 2	0.460 190 2	0.460 172 5	0.1
0.3	0.382 088 6	0.382 551 9	0.382 096 9	0.3
0.5	0.308 537 5	0.310 478 2	0.308 572 0	0.5001
1.0	0.158 655 3	0.168 573 8	0.158 808 0	1.0006
1.5	0.066 807 2	0.083 657 9	0.066 952 3	1.5011
2.0	0.022 750 1	0.039 485 4	0.022 701 2	1.9991
2.5	0.006 209 7	0.018 174 0	0.006 033 7	2.4901
3.0	0.001 349 9	0.008 266 0	0.001 212 5	2.9693
3.5	0.000 232 6	0.003 739 0	0.000 176 1	3.4332
4.0	0.000 031 7	0.001 687 1	0.000 017 6	3.8800

Figure 5.16 illustrates $\phi(x) - \alpha f_1(x)$ for $-3 \leq x \leq 3$, which may be simulated by means of rejection, the details of which are discussed in the

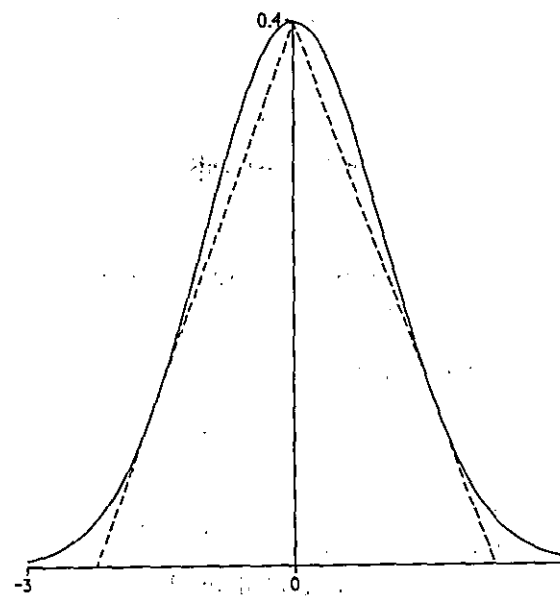


Figure 5.15 The standard normal density function $\phi(x)$ (—) over the range, $(-3, +3)$, and $\alpha f_1(x)$ (-----), in the notation of the composition method of the Section 5.4. Here $f_1(x)$ is the probability density function of $\beta(U_1 + U_2 - 1)$, where U_1 and U_2 are independent $U(0, 1)$ random variables. α is chosen so that $\alpha f_1(0) = 1/\sqrt{2\pi}$, and β must be chosen to give the triangle illustrated here, i.e. the largest symmetric triangle with height $1/\sqrt{2\pi}$ which can be fitted under $\phi(x)$.

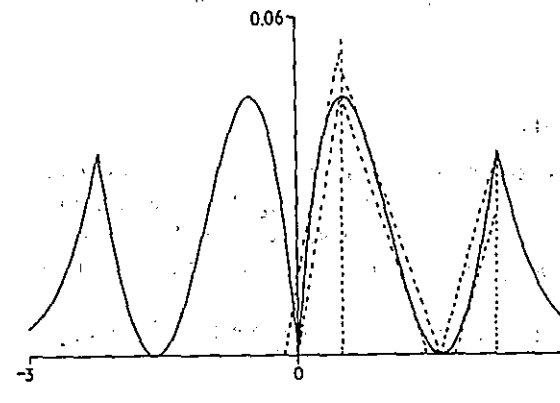


Figure 5.16 A graph of $\phi(x) - \alpha f_1(x)$ for $|x| \leq 3$, resulting from the curves of Fig. 5.15. The dotted lines relate to a particular approach used for the rejection method employed to simulate from the probability density function which is a positive multiple of this curve, as discussed in the solution to Exercise 5.38.

solution to Exercise 5.38. Also presented in Exercise 5.38 is the full algorithm of Kinderman and Ramage (1976).

5.8 Exercises and complements

(a) General

- 5.1 Use Equation (2.3) to show that when U is a $U(0, 1)$ random variable, then $1 - U$ is also a $U(0, 1)$ random variable.
- 5.2 When X has the half-normal p.d.f.

$$f_X(x) = \sqrt{\left(\frac{2}{\pi}\right)} e^{-x^2/2} \quad \text{for } x \geq 0$$

show that \tilde{X} , defined by:

$$\begin{cases} \tilde{X} = X & \text{with probability } \frac{1}{2} \\ \tilde{X} = -X & \text{with probability } \frac{1}{2} \end{cases}$$

has the standard normal p.d.f.

- 5.3 Simulating Poisson random variables with large mean can be time consuming, whether one uses a particular approach, as in Chapter 4, or a general, table-look-up approach. Discuss one way of tackling this problem, in the context of the distribution of the sum of two independent random variables, each with Poisson distributions. See Exercise 2.8(b).

(b) Table-look-up methods

- 5.4 Select a Poisson distribution with mode different from zero.
- Simulate from this distribution using the table-look-up method.
 - Repeat (a), but employ a θ , as suggested in Section 5.1.
 - Repeat (a) but employ two such θ 's, thus dividing the range into three parts.
 - Repeat (b) after having first ordered the probabilities in increasing order.
- Compare the efficiencies of these four approaches (cf. also Exercise 5.3, and Kemp, 1982).
- 5.5 (a) Write a computer program to simulate a random variable, X , from

the triangular distribution defined by:

$$f(x) = \begin{cases} 0 & x < 0 \\ x & 0 \leq x \leq 1 \\ 2-x & 1 \leq x \leq 2 \\ 0 & x > 2 \end{cases} \quad F(x) = \begin{cases} 0 & x < 0 \\ x^2/2 & 0 \leq x \leq 1 \\ 2x - (x^2/2) - 1 & 1 \leq x \leq 2 \\ 1 & x > 2 \end{cases}$$

using the inversion method. Here $f(x)$ is the probability density function of x , and $F(x)$ is the cumulative distribution function of x . This is the method used in the IMSL routine GGTRA (see Section A1.1).

- (b) Compare the efficiency of this program with one which simulates such a random variable by simply summing two independent $U(0, 1)$ random variables.
- 5.6 Use the table-look-up method to simulate 10 random variables:
- from the binomial distribution $B(6, 1/3)$; and
 - from the normal distribution $N(1, 2)$, using tables of the standard normal cumulative distribution function.
- *5.7 Use the table-look-up method to simulate random variables with the simple beta probability density function

$$f(x) = 6x(1-x) \quad \text{for } 0 \leq x \leq 1.$$

- *5.8 (a) Explain how to simulate random variables from the Cauchy distribution, with probability density function,

$$f(x) = \frac{1}{\pi(1+x^2)} \quad \text{for } -\infty \leq x \leq \infty$$

using the inversion method. An algorithm using this approach is provided by the IMSL routine, GGCAV (see Section A1.1).

- (b) If N_1 and N_2 are independent standard normal random variables then, as we saw in Exercise 2.15(b) and Exercise 4.5(b), their ratio $C = N_1/N_2$ has the Cauchy probability density function of (a) above. Explain how this result may be deduced from (a) and an understanding of the Box-Muller method described in Section 4.2.1.
- *5.9 The approximate approach for simulating $N(0, 1)$ random variables described in Section 5.7 involved setting $\tilde{x} = G^{-1}(u)$, where $G(x) = [1 + \exp\{-2a_1 x(1 + a_2 x^2)\}]^{-1}$. Solve for \tilde{x} .
- *5.10 Discuss how you would use the table-look-up method for simulating from the bivariate Poisson distribution of Exercise 4.7.

- *5.11 Discuss how you would use the inversion method for simulating from the bivariate normal distribution.
- 5.12 If X is a random variable with the exponential, $\lambda e^{-\lambda x}$ p.d.f., for $x \geq 0$, deduce the distribution of the integral part of X , viz., $Y = [X]$. Hence explain why, in (5.4), we obtain a geometric random variable by rounding up an exponential random variable.
- *5.13 Use the inversion method to simulate from the following distributions:

(a) logistic: $f(x) = \frac{e^{-x}}{(1+e^{-x})^2}$ for $-\infty \leq x \leq \infty$.

Note that this method is implemented in the NAG routine: GOSDCF (see Section A1.1).

(b) Weibull (see Exercise 2.3): $f(\omega) = \frac{\beta}{\gamma^\beta} \omega^{\beta-1} \exp\{-\omega/\gamma\}^\beta$ for $0 \leq \omega < \infty, \beta > 0, \gamma > 0$.

Note that this method is implemented in the NAG routine GOSDPF and the IMSL routine GGWIB (see Section A1.1).

(c) Pareto distribution:

$$\Pr(X \leq x) = 1 - \left(\frac{k}{x}\right)^a \quad \text{for } a > 0, x \geq k > 0.$$

(d) Extreme-value distribution:

$$\Pr(X \leq x) = \exp\{-\exp((\xi - x)/\theta)\} \quad \text{for } x \geq 0.$$

- 5.14 Provide a detailed algorithm for simulating from the logarithmic distribution of Exercise 4.22.
- *5.15 Barnett (1980) presents the bivariate uniform p.d.f.:

$$f(u, v) = (1 - \alpha)[(2uv - u - v)\alpha + 1]\{\Psi(u, v)\}^{-3/2} \quad (5.11)$$

where $\Psi(u, v) = (\alpha(u+v) - 1)^2 + 4\alpha(1 - \alpha)uv$ and $\alpha < 1, 0 \leq u, v \leq 1$. This probability density function is illustrated in Fig. 5.17 for the case $\alpha = -4$. It is constructed from a bivariate distribution of Plackett (1965), which is given implicitly by:

$$\frac{F(x, y)\{1 - F_x(x) - F_y(y) + F(x, y)\}}{\{F_x(x) - F(x, y)\}\{F_y(y) - F(x, y)\}} = 1 - \alpha$$

From Section 5.2 we can see that if we set $U = F_x(X)$ then U is $U(0, 1)$, and so is $V = F_y(Y)$. This is an interesting reversal of the aim of Section 5.2, which is to progress from U to X . Verify that this substitution here results in the joint p.d.f. $f(u, v)$ of Equation (5.11). Derive further bivariate uniform distributions in this manner from the following bivariate distributions also presented by Barnett (1980):

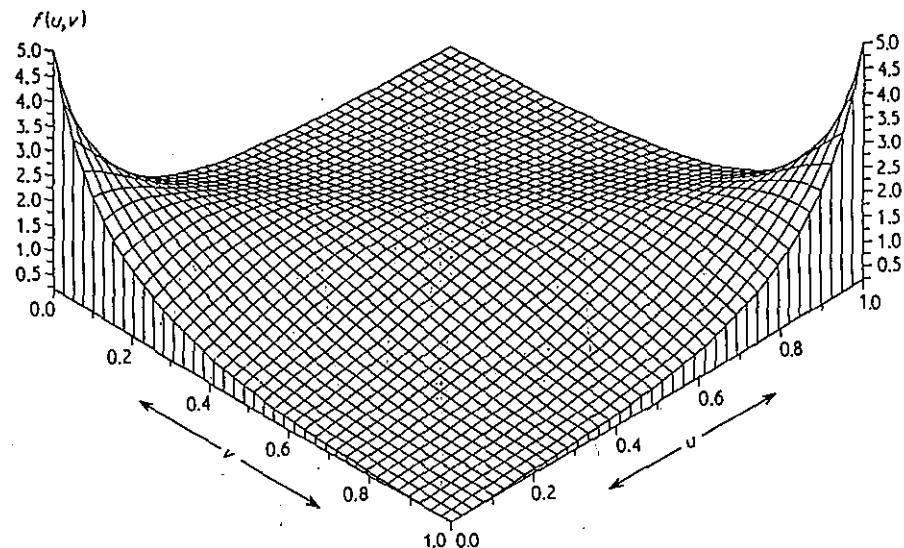


Figure 5.17 Isometric projection of the bivariate uniform density of Equation (5.11), from Morgan (1983).

(a) $F(x, y) = F_x(x)F_y(y)\{1 - \alpha(1 - F_x(x))(1 - F_y(y))\}$
for $|\alpha| < 1$.

(b) $f(x, y) = \{(1 + \alpha x)(1 + \alpha y) - \alpha\} \exp(-x - y - \alpha xy)$
for $0 < \alpha < 1$.

(this is a bivariate exponential distribution)

(c) $f(x, y) = \frac{1}{2\pi} (1 + x^2 + y^2)^{-3/2}$.

(this is a bivariate Cauchy distribution)

(c) Rejection methods

5.16. Figure 5.18 shows the probability density function $r(x)$ of Equation (5.10), resulting from the composition of (5.10). Explain how you would simulate from $r(x)$ using a rejection method.

5.17. To simulate from the probability density function given by:

$$f(x) = \begin{cases} \frac{1}{\pi \sqrt{1-x^2}}, & \text{for } -1 \leq x \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

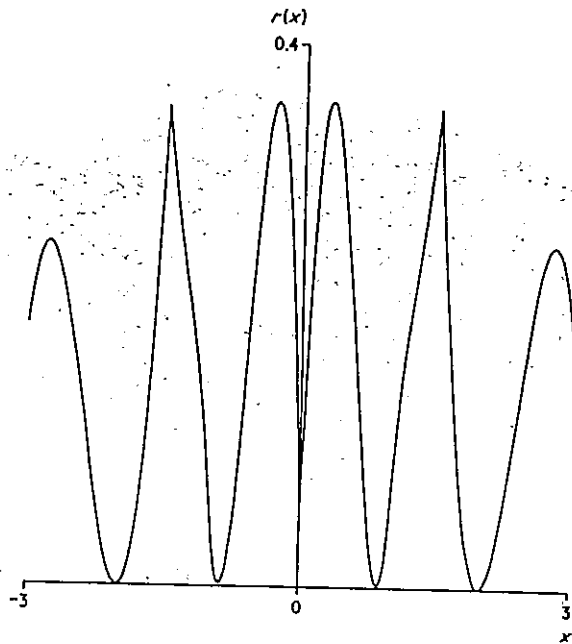


Figure 5.18 The p.d.f. $r(x)$ for $-3 \leq x \leq 3$, which is sampled with probability 0.0228 in the 'convenient' composition method of Equation (5.10).

we note that this is the probability density function of the random variable $X = \cos(\pi U)$, where U is a $U(0, 1)$ random variable. Use this result to devise a rejection method, based on the first quadrant of a circle and similar to the Polar Marsaglia method, for generating the required random variables.

- 5.18 Devise a rejection method, with an acceptance probability of not less than $8/9$, for simulating random variables from the beta probability density function $f(x) = 6x(1-x)$ for $0 \leq x \leq 1$.
- 5.19 Describe how to simulate a random variable with the logistic probability density function, $e^{-x}(1+e^{-x})^{-2}$ for $-\infty \leq x \leq \infty$, using a rejection method based on the exponential envelope, e^{-x} for $x \geq 0$.
- 5.20 Explain how to simulate normal random variables using a rejection method with an enveloping function based on a logistic p.d.f. Derive the probability of rejection (cf. Exercise 5.31).
- 5.21 Repeat the approach adopted in Example 5.5 with $k\lambda e^{-\lambda x}$ for $x \geq 0$ as the enveloping function. Show that the probability of rejection is minimized if we take $\lambda = 1$, as in Example 5.5.

- *5.22 Cheng (1977) presented a rejection method for simulating from the $\Gamma(\alpha, 1)$ distribution, where $\alpha > 1$. In his case,

$$h(x) = \lambda \mu x^{\lambda-1} (\mu + x^\lambda)^{-2} \quad \text{for } x \geq 0$$

- (a) Consider how you would simulate from the probability density function, $h(x)$.
- (b) If $\mu = \alpha^2$ and $\lambda = \sqrt{2\alpha - 1}$, determine the probability of rejection, and the mean number of variable selections until acceptance. The case $\alpha = 3$ is illustrated in Fig. 5.5, for $x < 8$.
- *5.23 Compare the two rejection methods for simulating from a gamma distribution, given in Example 5.6 and Exercise 5.22.
- *5.24 Explain how you would simulate a random variable that has an exponential distribution of mean 2, conditional on it being greater than 9 (cf. Exercise 5.26).
- *5.25 Figure 5.16 presents a p.d.f. to be simulated from by means of a rejection method. Kinderman and Ramage (1976) used the method of triangles (see Marsaglia, MacLaren and Bray, 1964), which, in outline, is as follows.

If a p.d.f. from which one wants to simulate can be sandwiched between two parallel lines, the X -value for the rejection method is simulated from an appropriate triangular distribution corresponding to the upper of the parallel lines. When the corresponding uniformly distributed Y value is less than the appropriate value on the lower of the parallel lines, then X is accepted, and it is not necessary to compute the formula for the curve. If, however, the Y value is greater than the appropriate value on the lower line then it is necessary to compute the formula for the curve in order to decide on rejection or acceptance.

Discuss the objective of such an approach, and explain its use for the beta p.d.f. of Exercise 5.18 (cf. comments in the solution to Exercise 5.23).

- *5.26 Marsaglia (1964) proposed the following method for simulating standard normal random variables X , conditional upon $X > a > 0$. Let U_1, U_2 be two independent $U(0, 1)$ random variables. Set

$$X = (a^2 - 2 \log_e U_1)^{1/2}.$$

Accept X as a realization of the required random variable if $U_2 X < a$. Otherwise, reject U_1 and U_2 , and start again. Verify that X has the required distribution (cf. Exercise 5.24 and the comments of Section 5.5).

- *5.27 If U_1 and U_2 are independent $U(0, 1)$ random variables, show that,

conditional upon $(2U_1 - 1)^2 + U_2^2 \leq 1$, then $C = (2U_1 - 1)/U_2$ has the Cauchy distribution of Section 2.11. Note that this method is implemented in the NAG routine G05DFF (see Section A1.1).

5.28 If X_1 and X_2 are independent, identically distributed exponential random variables with mean unity, show that, conditional upon $(X_1 - 1)^2 < 2X_2$, then X_1 has a half-normal p.d.f., derived from an $N(0, 1)$ distribution. (This result is due to von Neumann—see Kahn, 1956, p. 39.)

*5.29 Suppose we have a probability density function $f(x)$ which can be written in the form:

$$f(x) = cg(x)r(x)$$

where $g(x)$ is also a p.d.f., $c > 0$ is a constant, and over the range of x , $0 \leq r(x) \leq m$, for some finite m . Show that we can simulate X from $f(x)$ as follows:

- (i) Simulate X from $g(x)$
- (ii) Accept X if $Um < r(X)$

where U is an independent $U(0, 1)$ variable. Otherwise reject X and U and start again at (i).

What is the rejection probability? An example is provided by Butcher (1960), in which $f(x)$ is half-normal, and $g(x)$ is exponential. This generalization of the rejection method can give rise to efficient 'switching' algorithms, in which the rôles played by $g(x)$ and $r(x)$ change for different parts of the x -range; see Atkinson and Whittaker (1976), and Atkinson (1979b).

(d) Composition methods

†5.30 Use the composition approach of Section 5.4, as applied in the example of Equation (5.6), to simulate random variables with the Poisson distribution of Example 5.2.

5.31 Explain why it is not possible to simulate normal random variables using a composition, the first element of which, $f_1(x)$, is a logistic density.

†5.32 A continuous random variable X has the 'wedge-shaped' probability density function, $f_1(x) = \alpha - \alpha^2 x/2$, for $0 \leq x \leq 2/\alpha$ and $\alpha > 0$.

- (a) Explain how you would simulate X .
- (b) It is desired to simulate from the exponential p.d.f. $f(x) = \lambda e^{-\lambda x}$ for $x \geq 0$ and $2\lambda > \alpha$, using a composition, the first p.d.f. of which is to be $f_1(x)$. Derive the shrinking factor for $f_1(x)$, and deduce that, by

suitable choice of α , the probability of simulating from $f_1(x)$ in the composition can be made as large as $2/e$.

5.33 (a) Show that the random variable X , with probability density function

$$f(x) = \frac{e^{m-x}}{(e-1)} \quad \text{for } (m-1) < x \leq m, \text{ where } m \geq 1$$

is obtained simply by setting $X = m - Y$, where Y has probability density function

$$f(y) = \frac{e^y}{(e-1)} \quad \text{for } 0 \leq y < 1$$

The cumulative distribution function for X when $m = 1$ is illustrated in Fig. 5.2.

(b) By expanding $f(y)$ as a power series in y , show that we can simulate from $f(y)$ by means of a composition, simulating from probability density function, $(i+1)y^i$ for $0 \leq y < 1$, with probability

$$\frac{1}{(i+1)!(e-1)} \quad \text{for } i \geq 0.$$

5.34 (continuation) We note that

$$e^{-x} = \frac{(e-1)e^{-m} \times e^{m-x}}{(e-1)} \quad \text{for any } m \geq 1$$

Explain, with reference to Fig. 5.19, how this result may be used as a basis for a composition method for simulating from the probability density function, e^{-x} for $x \geq 0$.

*5.35 (continuation) Explain the following algorithm, given by Marsaglia (1961), for simulating random variables from the exponential e^{-x} p.d.f.:

(i) Simulate a discrete random variable, I , from the distribution

$$\frac{1}{(i+1)!(e-1)} \quad \text{for } i \geq 0$$

(ii) Set $W = \max(U_1, U_2, \dots, U_{I+1})$, where the $\{U_j\}$ are independent $U(0, 1)$ random variables.

(iii) Simulate a discrete random variable, M , from the distribution

$$(e-1)e^{-m} \quad \text{for } m \geq 1$$

(iv) Set $X = M - W$.

*5.36 Consider how you would simulate standard normal random variables using a composition method, in which the first p.d.f. in the composition, $f_1(x)$, is of trapezoidal form. See Ahrens and Dieter (1972) for an algorithm based on this approach.

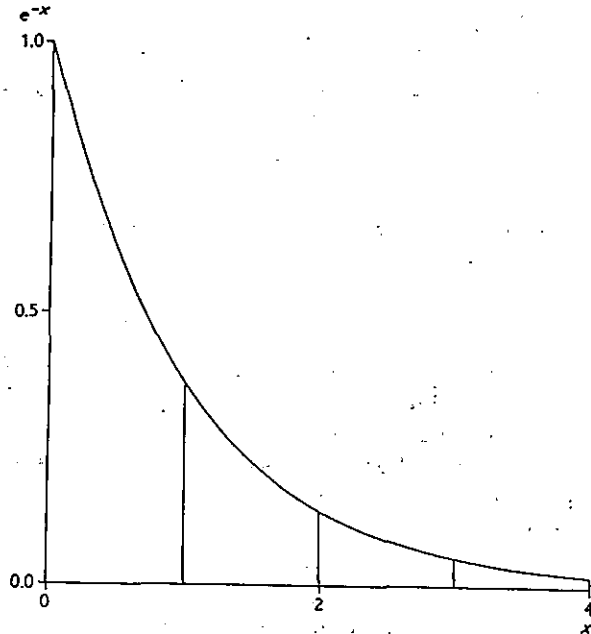


Figure 5.19 A breakdown of the p.d.f. e^{-x} into sections of area, $(e-1)e^{-m}$, for $m \geq 1$, for $x \leq 4$.

*5.37 Figure 5.20 illustrates a portion of the half-normal p.d.f. $2\phi(x)$, and $0.97f_1(x)$, in which $f_1(x)$ is a density composed of 97 rectangles, each of area $1/97$. Figure 5.21 illustrates $2\phi(x) - 0.97f_1(x)$. Discuss how these curves may be used to simulate standard normal random variables. This method is due to Leden-Hitchcock (1980) and is based on a method of Marsaglia, MacLaren and Bray (1964).

*5.38 Kinderman and Ramage (1976) produce the algorithm, given below, for their method discussed in Section 5.7. Explain how the method gives rise to this algorithm. (Note that $\xi = 2.216035867166471$ and $f(t) = \phi(t) - 0.18025191068563(\xi - |t|)$, for $|t| < \xi$. Here we preserve the high accuracy of constants given in the original source.)

Algorithm from Kinderman and Ramage (1976)

1. Generate u . If $u < 0.884070402298758$, generate v and return $x = \xi \times (1.131131635444180u + v - 1)$.
2. If $u < 0.973310954173898$, go to 4 below.
3. Generate v, w . Set $t = \xi^2/2 - \log_e w$. If $v^2 t > \xi^2/2$, begin this step

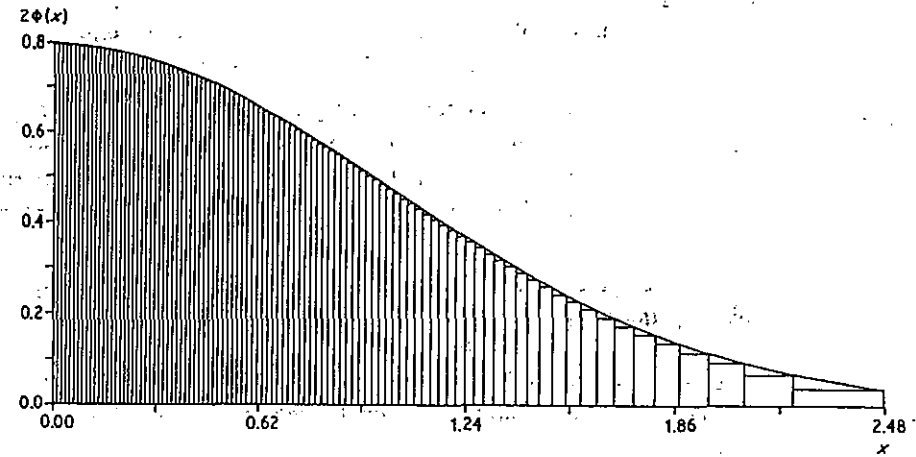


Figure 5.20 Part of the half-normal density,

$$2\phi(x) = \sqrt{\left(\frac{2}{\pi}\right)} e^{-x^2/2},$$

enveloping 97 rectangles, each of area 0.01.

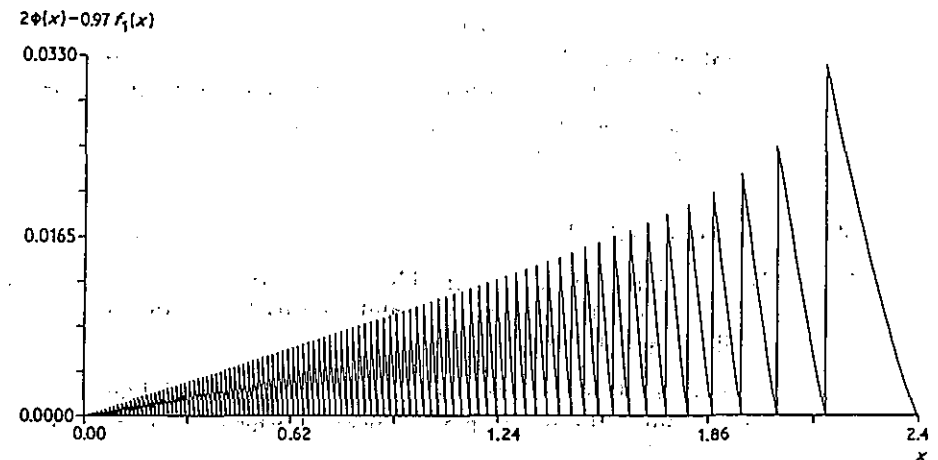


Figure 5.21 A graph of $2\phi(x) - 0.97f_1(x)$, from Fig. 5.20, in which $0.97f_1(x)$ is the envelope of the rectangles shown in Fig. 5.20.

again. Otherwise return $x = (2t)^{1/2}$ if $u < 0.986655477086949$ or return $x = -(2t)^{1/2}$ if not.

4. If $u < 0.958720824790463$, go to 6 below.
5. Generate v, w . Set $z = v - w$ and $t = \xi - 0.630834801921960 \times$

$\min(v, w)$. If $\max(v, w) \leq 0.755\ 591\ 531\ 667\ 601$, go to 9. If $0.034\ 240\ 503\ 750\ 111 |z| \leq f(t)$, go to 9. Otherwise, repeat this step.

6. If $u < 0.911\ 312\ 780\ 388\ 703$, go to 8.

7. Generate v, w . Set $z = v - w$ and

$$t = 0.479\ 727\ 404\ 222\ 441 + 1.105\ 473\ 661\ 022\ 070 \min(v, w).$$

If

$$\max(v, w) \leq 0.872\ 834\ 976\ 671\ 790$$

go to 9. If $0.049\ 264\ 496\ 373\ 128 |z| \leq f(t)$ go to 9. Otherwise, repeat this step.

8. Generate v, w . Set $z = v - w$ and

$$t = 0.479\ 727\ 404\ 222\ 441 - 0.59550\ 71380\ 15940 \min(v, w).$$

If

$$\max(v, w) \leq 0.805\ 577\ 924\ 423\ 817$$

go to 9. If $0.053\ 377\ 549\ 506\ 886 |z| \leq f(t)$, go to 9. Otherwise, repeat this step.

9. If $z < 0$, return $x = t$; otherwise return $x = -t$.

*5.39 For the residual p.d.f. $r(x)$ from the composition of Equation (5.10), show that the probability of rejection is 0.53 when we simulate from $r(x)$ using rejection and an enveloping rectangle.

(e) Additional methods

*5.40 Suppose W is $U(a, b)$, for some $b > a$, and suppose that for $a \leq x \leq b$, $0 \leq g(x) \leq 1$ for some function $g(x)$. Suppose N is the first integer ≥ 1 such that

$$g(W) \geq U_1 \geq U_2 \geq \dots \geq U_{N-1} < U_N$$

where the $\{U_i\}$ are a sequence of independent, identically distributed $U(0, 1)$ variables. Thus $N = 1$, if and only if $g(W) < U_1$

$$N = 2, \text{ if and only if } g(W) \geq U_1 < U_2$$

etc.

Show that

$$\Pr(N = n | W = w) = \frac{g(w)^{n-1}}{(n-1)!} - \frac{g(w)^n}{n!} \quad \text{for } n \geq 1$$

and deduce that

$$\Pr(N \text{ is odd} | W = w) = \exp(-g(w))$$

Finally, show that the conditional p.d.f. of W is given by

$$f_W(w | N \text{ is odd}) = \frac{\exp(-g(w))}{\int_a^b \exp(-g(w)) dw} \quad (5.12)$$

*5.41 (continuation) Use the results of the last exercise to provide a rejection method to simulate random variables with the p.d.f. of Equation (5.12) over the range (a, b) . This is the basis of what is known as Forsythe's method (see Forsythe, 1972), which has been used for a variety of distributions (see Atkinson and Pearce, 1976). Of course, the requirement that $g(x) \leq 1$ is, by itself, very restrictive; however, this restriction can be overcome by dividing up the range of x into a number of intervals, and then first of all using a composition to determine the appropriate interval: if $\bar{g}(x)$ is an increasing function of x , over the range $(0, \infty)$, say, then if the interval (q_i, q_{i+1}) is chosen by the first stage of the composition method, $\{\bar{g}(q_i + x) - \bar{g}(q_i)\}$ plays the rôle of $g(x)$ in the last exercise. The $\{q_i\}$ must be chosen so that

$$0 \leq \bar{g}(q_i + x) - \bar{g}(q_i) \leq 1 \quad \text{for } 0 \leq x \leq (q_{i+1} - q_i)$$

One such choice of $\{q_i\}$ gives rise to what is called Brent's GRAND method for $N(0, 1)$ variables (see Brent, 1974). This is the method employed by the NAG routine, GOSDDF (see Section A1.1). Further discussion and comparisons with other methods are given by Atkinson and Pearce (1976). One advantage of Forsythe's method is that it avoids time-consuming exponentiation.

*5.42 The random variable X takes the values 1, 2, 3, 4 with the following probabilities:

$$\Pr(X = 1) = \frac{1}{6} = \frac{1}{4}(\frac{2}{3} + 0 + 0 + 0)$$

$$\Pr(X = 2) = \frac{1}{12} = \frac{1}{4}(0 + \frac{1}{3} + 0 + 0)$$

$$\Pr(X = 3) = \frac{7}{12} = \frac{1}{4}(\frac{1}{3} + \frac{2}{3} + 1 + \frac{1}{3})$$

$$\Pr(X = 4) = \frac{1}{6} = \frac{1}{4}(0 + 0 + 0 + \frac{2}{3})$$

Thus, by analogy with Equation (5.6), we can write

$$\Pr(X = i) = \frac{1}{4} \sum_{j=1}^4 r_{ij}$$

where the $\{r_{ij}, 1 \leq i \leq 4\}$ are all probability distributions, for each j , $1 \leq j \leq 4$. The difference as compared with Equation (5.6) is that now random variables with any of the four $\{r_{ij}, 1 \leq i \leq 4\}$ distributions take just one of at most two values, and the distributions in the composition have equal probability of being used. Show that any discrete random

variable X over a finite range can be obtained by means of such a composition (Kronmal and Peterson, 1979). This composition results in the *alias* method, so called because if the $\{r_{ij}, 1 \leq i \leq 4\}$ distributions do not select the value $X = j$ then the 'alias' value for X is chosen by the $\{r_{ij}, 1 \leq i \leq 4\}$ distribution. For example, in the above illustration, with probability $\frac{1}{4}$ the component distribution, $\{r_{i2}, 1 \leq i \leq 4\}$ is selected, and then either $X = 2$, with probability $r_{22} = \frac{1}{3}$, or $X = 3$, the alias value, with probability $r_{23} = \frac{2}{3}$. For further discussion, see Peterson and Kronmal (1982). An attractive feature of this method is that it does not require more than two uniform random variables for each value of X . Can you suggest a way in which only one uniform random variable need be used? (See Kronmal and Peterson, 1979.) An algorithm for the alias method is provided by the IMSL routine GGDA (see Section A1.1).

6

TESTING RANDOM NUMBERS

6.1 Introduction

The need for stringent testing of uniform random variables was emphasized in Chapter 3. When tables of random digits were first produced, tests were employed for uniform random digits. More recently, with the development of pseudo-random-number generators, the numbers to be tested are continuously distributed over the range $(0, 1)$. In the latter case, tests for digits are frequently applied to the digit occupying the first decimal place, while in some cases of detailed testing other decimal places are also considered, as in Wichmann and Hill (1982a). An alternative approach, given by Cugini *et al.* (1980), is described in Section 6.3.

We have seen that congruential methods of random number generation are convenient and widely used, but that they can produce sequences of numbers with certain undesirable properties. For any particular application, the need is to determine what may be 'undesirable', so that random numbers should always be tested with an application in mind. This is often easier said than done, but we can see that it could entail testing not only uniform variables, but also variables of other distributions, obtained by methods such as those of the last two chapters. In Chapter 5 in particular, some of the algorithms given are very complicated, and in such cases testing is needed quite simply as a check that there have been no programming errors. In Chapter 4 we saw that particular properties of random variables and processes can be used to generate particular random variables. By the same token, similar properties may be used to test particular random variables, as we shall see in Section 6.6.

A room full of eternally typing monkeys will ultimately produce the plays of Shakespeare, and similarly, a large enough table of uniform random digits will, by the very nature of random digits, contain sections which, by themselves, will certainly fail tests for uniformity. This feature is noted in the table of Kendall and Babbington-Smith (1939a), which contains 100 000 digits. They tested their table as a whole, and also in parts, down to blocks of 1000 digits each. As

Ref (2)
11
✓

variable X over a finite range can be obtained by means of such a composition (Kronmal and Peterson, 1979). This composition results in the *alias* method, so called because if the $\{r_{ij}, 1 \leq i \leq 4\}$ distributions do not select the value $X = j$ then the 'alias' value for X is chosen by the $\{r_{ij}, 1 \leq i \leq 4\}$ distribution. For example, in the above illustration, with probability $\frac{1}{4}$ the component distribution, $\{r_{i2}, 1 \leq i \leq 4\}$ is selected, and then either $X = 2$, with probability $r_{22} = \frac{1}{3}$, or $X = 3$, the alias value, with probability $r_{23} = \frac{2}{3}$. For further discussion, see Peterson and Kronmal (1982). An attractive feature of this method is that it does not require more than two uniform random variables for each value of X . Can you suggest a way in which only one uniform random variable need be used? (See Kronmal and Peterson, 1979.) An algorithm for the alias method is provided by the IMSL routine GGDA (see Section A1.1).

6 TESTING RANDOM NUMBERS

6.1 Introduction

The need for stringent testing of uniform random variables was emphasized in Chapter 3. When tables of random digits were first produced, tests were employed for uniform random digits. More recently, with the development of pseudo-random-number generators, the numbers to be tested are continuously distributed over the range (0, 1). In the latter case, tests for digits are frequently applied to the digit occupying the first decimal place, while in some cases of detailed testing other decimal places are also considered, as in Wichmann and Hill (1982a). An alternative approach, given by Cugini *et al.* (1980), is described in Section 6.3.

We have seen that congruential methods of random number generation are convenient and widely used, but that they can produce sequences of numbers with certain undesirable properties. For any particular application, the need is to determine what may be 'undesirable', so that random numbers should always be tested with an application in mind. This is often easier said than done, but we can see that it could entail testing not only uniform variables, but also variables of other distributions, obtained by methods such as those of the last two chapters. In Chapter 5 in particular, some of the algorithms given are very complicated, and in such cases testing is needed quite simply as a check that there have been no programming errors. In Chapter 4 we saw that particular properties of random variables and processes can be used to generate particular random variables. By the same token, similar properties may be used to test particular random variables, as we shall see in Section 6.6.

A room full of eternally typing monkeys will ultimately produce the plays of Shakespeare, and similarly, a large enough table of uniform random digits will, by the very nature of random digits, contain sections which, by themselves, will certainly fail tests for uniformity. This feature is noted in the table of Kendall and Babbington-Smith (1939a), which contains 100 000, digits. They tested their table as a whole, and also in parts, down to blocks of 1000 digits each. As

expected, some of these individual blocks failed certain tests, and a note was added to these blocks, to 'caution the reader from using them by themselves'.

EXAMPLE 6.1

As an illustration of this, let us consider the digits of Table 3.1. For the two halves of the table we obtain the following frequencies for single digits:

Digit	0	1	2	3	4	5	6	7	8	9	Totals
(a)	17	16	13	16	17	16	36	16	20	13	180
(b)	15	19	20	19	14	22	16	20	11	24	180
(a) + (b)	32	35	33	35	31	38	52	36	31	37	360

For the entire table, if the digits were random the expected number for each digit is $360/10 = 36$, and so the departures from 36 observed can be tested by the chi-square test of Section 2.14. Here no parameters have been estimated from the data, and so the number of degrees of freedom is 9. For the entire table we obtain $\chi^2_9 = 9.39$, which is not significant at the 5% level. However, if we take part (a) of the table above, we find $\chi^2_9 = 22$, just significant at the 1% level, for a one-tail significance test, or the 2% level for a two-tail test. As we shall see later, two-tail tests are frequently used for testing random numbers.

In the context of pseudo-random numbers, we have already encountered this same point in Chapter 3, since congruential generators can be devised which have a low first-order serial correlation for their full cycle, but which result in much higher such correlations for fractions of the cycle (see Exercise 6.1). A property of a pseudo-random number generator for its entire cycle provides, effectively, a test of that generator, and a test of a kind that is not possible for physical random number generators. As well as serial correlations, the first- and second-order moments of Exercise 3.13 can be interpreted in this way. Such tests have come to be known as *theoretical* tests, and an elaborate such test is the *spectral test* of Coveyou and MacPherson (1967). Theoretical tests evaluate the generating mechanisms used, and do not make use of generated numbers. Knuth (1981, p. 89) states that all congruential generators that are thought to be good pass the spectral test, while those that are known to be bad fail it. Oakenfull (1979) and Knuth (1981, p. 102) provide the results of applying this test to a variety of congruential generators. Ultimately, however, we have to test the numbers produced by a generator in the context of their use, and this is done by a variety of *empirical* tests, which are the subject of this chapter. Atkinson (1980) describes when the spectral test is appropriate, and for a number of generators compares the results of theoretical and empirical

tests. The same theoretical/empirical comparison is also made by Grafton (1981).

6.2 A variety of tests

When we are dealing with random variables such as Poisson or normal, we want to check that the generated values come from the distributions we think they do. In the case of Poisson variables this could involve checking that the differences between the bar-charts of Fig. 2.3, for example, are not significant, while for normal variables we would be comparing, for instance, the density function of Fig. 2.5(a) with the histogram of Fig. 2.5(b). Methods for making these comparisons will be considered later. In addition, we may well want to consider the serial dependence of the variables, as is done for instance by Barnett (1965) for exponential random variables. Obvious discrepancies can sometimes be spotted by inspection of a convenient graphical display, as can be done for the figures of Chapter 2, but ultimately significance tests must be applied. The scatter plot of Fig. 3.2 is 'obviously' non-random, but what can we say of the scatter of Fig. 3.3? The same question can be asked of the plot of Fig. 6.1, produced by the generator of Equation (3.1).

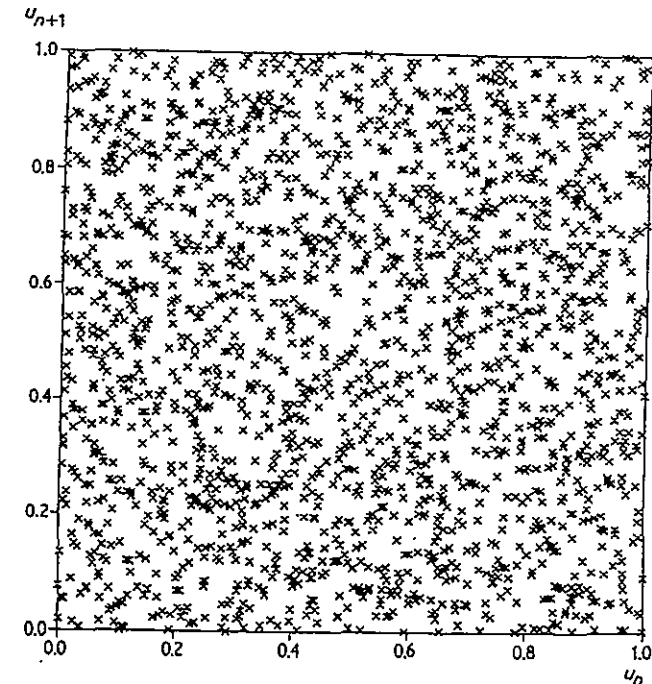


Figure 6.1 A scatter plot of u_{n+1} vs. u_n for a sequence of length 2000 from the generator of Equation (3.1).

Recently a sophisticated approach to judging the randomness of scatter plots has been provided by Ripley (1977, 1981), whose technique itself utilizes repeated simulations, and Atkinson (1977b) applied this technique to numbers resulting from the multiplicative congruential generator

$$x_{i+1} = 5x_i$$

discussed earlier in Equation (3.4).

In inspecting and testing scatter plots such as that of Fig. 6.1, we are implicitly considering how often different one- and two-dimensional intervals are represented. This corresponds to the basic frequency and serial tests which we shall soon describe. Apart from these, however, what other empirical tests should we apply? Thus, hard on the heels of the earlier problems of generator selection and, when appropriate, which method to use for transforming uniform random variables, is the problem of test selection. As mentioned earlier, the glib answer is that tests should be suggested by the use intended for the random variables, and this could result in the application of very specific tests, over and above those already applied to a basic source generator. Different producers of uniform random numbers have answered this question in different ways, and batteries of tests are to be found, for example, in Kendall and Babbington-Smith (1939), Tausky and Todd (1956), Craddock and Farmer (1971), Miller and Prentice (1968) and Wichmann and Hill (1982a).

It is important to realize that there is nothing magical or God-given about a particular set of tests. Clearly an infinity of tests is possible, and as we shall see, numbers which pass one test may fail another. Kendall and Babbington-Smith used just four tests, designed to check frequencies and various forms of sequential dependence, and this basic approach is that adopted by subsequent authors, though conventions have changed with time. We shall now describe certain standard tests for uniform random digits, and then see the results of applying these tests to sequences resulting from a variety of generators.

6.3 Certain tests for uniform random digits

When presented with tables of digits such as those of Tables 3.1, 3.2 and Exercise 3.10, the first reaction of most of us would be to count up the frequencies of occurrence of each digit and compare the observed frequencies with what we would expect for random digits. The statistical yardstick that is usually used in making this comparison is the chi-square test of Section 2.14, and we have already seen such examples of a frequency test in Example 6.1, and Exercise 2.24.

Deterministic sequences such as: ... 89012345678901 ... satisfy the

frequency test (if a one-tail test is used — see later), but blatantly fail tests which consider the ordering of the elements in the sequence. The simplest such test, the serial test, takes a sequence of digits: ... $d_i, d_{i+1}, d_{i+2}, \dots$, and from considering non-overlapping pairs of digits compares the observed matrix $\{O_{kl}\}$ with the expected $\{e_{kl}\}$, $0 \leq k, l \leq 9$, in which digit l is observed to follow digit k , O_{kl} times, and e_{kl} is the corresponding number to be expected if we have a truly random sequence. If we have n non-overlapping pairs of digits, then $e_{kl} = n/100$, for $0 \leq k, l \leq 9$. The yardstick here is again a chi-square test, but this time on 99 degrees of freedom. An illustration of a serial test is given in Example 6.2.

Non-overlapping pairs of digits are taken so that the independence requirement of the chi-square test is preserved (see Section 2.14). If overlapping pairs are used, then a modified test, due to Good (1953), may be used. The IMSL routine GTPST, of Section A1.2 performs this test. It is an interesting footnote that Kendall and Babbington-Smith (1939a) used overlapping pairs and then incorrectly applied the standard chi-square test. Deterministic sequences such as that illustrated above do in fact produce *too good* an agreement with expectation in the frequency test, and this is indicated by significantly small values of the chi-square goodness-of-fit statistic. Consequently, chi-square tests of randomness are often two-tail tests, unlike customary chi-square tests in which only the upper tail is used as the critical region. An example of a sequence of digits that are too regular is provided by the first 2000 decimal digits of $e = 2.71828 \dots$. Here the frequency test gives $\chi^2_9 = 1.06$, a value which is significant at the 0.2% level, using a two-tail test. If the first 10 000 decimal digits of e are taken, then we obtain the satisfactory result: $\chi^2_9 = 8.61$; a more detailed breakdown can be found in Stoneham (1965), some of whose results are illustrated in Example 6.7 and Exercise 6.15.

Of course, as stated in Section 2.14, the chi-square test is an asymptotic test, and so is not appropriate if expected cell values are 'small'. The serial test generalizes to the consideration of triples, quadruples and so on, of digits, and the number of cells correspondingly increases geometrically. Thus, especially if one is considering non-overlapping n -tuples, care must be taken in tests of high-dimensional randomness to ensure that expected cell values are large enough for the chi-square test to be valid. An alternative test of randomness in high-dimensional space is the collision test described by Knuth (1981, pp. 68–70), and for which a FORTRAN program is given by Hopkins (1983b).

We can test random digits in a less routine way, by looking for patterns. One rudimentary way of doing this is provided by the gap test, which is as follows: select any digit, e.g. 7. We can now consider any sequence as consisting of 7's and 'not 7's', i.e., a binary sequence in which $\text{Pr}(7) = 1/10$, and $\text{Pr}(\text{not } 7) = 9/10$, if the sequence is random, and if successive digits are independent then the distribution of the number of digits between 7's is geometric (see

Section 2.6). Thus empirical and observed distributions of numbers of digits between 7's may be compared. For an illustration, see Example 6.2. Like the gap test, the 'coupon-collector' test is also based on a waiting-time, as it considers the number of digits until at least one of each of the digits 0-9 has appeared. This test treats all digits equally, and was first proposed by Greenwood (1955), who found that the test was satisfied by the first 2486 digits in the decimal expansion of $e = 2.71828 \dots$ and by the first 2035 digits in the decimal expansion of $\pi = 3.14159 \dots$; details of his test results can be found in Exercise 6.7.

A more obvious way of looking for patterns is provided by the *poker* test, which considers digits in sequences of length 5, and classifies the patterns according to the conventions of the game of poker: all different, two pairs, etc. Further discussion of the coupon-collector and poker tests is provided in Exercises 6.6, 6.7 and 6.15, and Example 6.7. The poker test may be performed by means of the IMSL routine - GTPOK (see Section A1.2).

Example 6.2 gives the results of applying the serial and gap tests to sequences produced by the random number generator of the Commodore PET microcomputer. This generator is not of a standard form, and will not be described here.

EXAMPLE 6.2 *The result of applying the serial and gap tests to the Commodore PET microcomputer random number generator*

(a) SERIAL TEST:

	Following value											Totals	
	1	2	3	4	5	6	7	8	9	10	11		
Preceding value	1	15	17	18	27	20	16	21	18	21	20	14	207
	2	30	24	20	18	25	13	18	24	27	25	17	241
	3	25	18	19	23	28	15	14	16	16	16	22	212
	4	14	24	23	14	22	16	17	16	18	19	19	202
	5	24	16	16	15	15	23	17	21	24	23	18	212
	6	22	24	22	27	18	8	17	19	31	24	25	237
	7	26	22	21	15	19	24	13	20	19	19	17	215
	8	24	13	18	26	21	16	19	21	19	14	20	211
	9	14	17	24	22	18	18	17	15	18	18	21	202
	10	22	24	26	27	23	25	18	23	25	16	23	252
	11	22	13	24	25	26	18	21	18	25	14	23	229
Totals	238	212	231	239	235	192	192	211	243	208	219	2420	

Here we obtain $\chi^2_{120} = 108.8$, which is clearly not significant, and so on the basis of this test we would not reject the hypothesis that the digits were uniform and random.

(b) GAP TEST

Gap size	Actual count	Expected count
0	36	25.90
1	36	23.31
2	23	20.98
3	20	18.88
4	17	16.99
5	6	15.29
6	15	13.76
7	10	12.39
8	11	11.15
9	10	10.03
≥ 10	75	90.31
Totals	259	258.99

Here $\chi^2_{10} = 19.924$, which is close to significance at the 5% level (two-tail test), and one would want to repeat this test to see if other samples produced similar results.

Note that these and other test results presented later in this chapter were obtained using the suite of BASIC test programs of Cugini *et al.* (1980). Rather than work with digits, they divided the (0, 1) interval into 11 sections for the serial test, while for the gap test, gaps were recorded between numbers lying in the (0.03, 0.13) interval. Thus for the gap test,

$$25.90 = 259/10,$$

$$23.31 = 25.9 \times 0.9, \text{ etc.}$$

*6.4 Runs tests

A striking feature of a table of digits can be the occurrence of *runs of the same digit*. If such runs occur with greater frequency than one would expect for random digits then one might, for example, expect this feature to result in a significant departure from the geometric distribution of the gap test. One can, however, look at distributions of other types of runs, and this was done by Downham and Roberts (1967).

Runs tests are frequently applied to a sequence of $U(0, 1)$ variates. Here we shall just consider 'runs up'. To illustrate what is meant by a 'run up', consider the following sequence of numbers, given here to 3 decimal places:

$$(0.134 \ 0.279 \ 0.886) (0.197) (0.011 \ 0.923 \ 0.990) (0.876)$$

The 'runs up' are indicated in parentheses, so that here we have four such runs, of lengths 3, 1, 3, 1, respectively. We see that a 'run up' ends when the next item

in the sequence is less than the preceding item, the next item then starting the next 'run-up'. Levene and Wolfowitz (1944) showed that in a random sequence of n $U(0, 1)$ variates, the expected number of 'runs up' of length $k \geq 1$, R_k , say, is given by:

$$E[R_k] = \frac{(k^2 + k - 1)(n - k - 1)}{(k + 2)!} \quad \text{for } 1 \leq k \leq n$$

(See also Knuth, 1981, pp. 65-68, for a derivation of this result.)

Typically, n is taken to be large, so that

$$E[R_k] \approx \frac{(k^2 + k - 1)}{(k + 2)!} n \quad \text{for } k \ll n$$

Clearly, for fixed n , $E[R_k]$ decreases as $k \rightarrow n$, and it is usual to consider the joint distribution of $(R_1, R_2, \dots, R_j, S_j)$, for some $j > 1$, where $S_j = \sum_{k=j+1}^n R_k$; $j = 5$ is frequently adopted. Successive run lengths are not independent, and so a standard chi-square test for comparing observed and expected numbers of runs is inappropriate. The test-statistic used (see Levene and Wolfowitz, 1944) is

$$U = \frac{1}{n} \sum_{i=1}^6 \sum_{j=1}^6 (X_i - E[X_i])(X_j - E[X_j])a_{ij} \quad (6.1)$$

in which $X_k = R_k$ for $1 \leq k \leq 5$, and $X_6 = S_6$,

the $\{a_{ij}\}$ form the inverse of the variance-covariance matrix of the $\{X_k\}$, and for large n are given by:

$$A \approx \begin{pmatrix} 4529.4 & 9044.9 & 13568 & 18091 & 22615 & 27892 \\ & 18097 & 27139 & 36187 & 45234 & 55789 \\ & & 40721 & 54281 & 67852 & 83685 \\ & & & 72414 & 90470 & 111580 \\ & & & & 113262 & 139476 \\ & & & & & 172860 \end{pmatrix}$$

the lower half of this matrix being obtained from symmetry. The exact expression is given by Knuth (1981, p. 68). U is referred to chi-square tables on 6 (not 5) degrees of freedom. As with the usual chi-square test, an asymptotic approximation is being made when this test is used, and Knuth recommends taking $n \geq 4000$. An illustration of the outcome of applying this test is given in the following example.

EXAMPLE 6.3 The result of applying the 'runs up' test to a sequence of length $n = 5000$ from the generator $(131, 0; 2^{35})^\dagger$

[†] Note that for convenience we shall henceforth use the notation: $(a, b; m)$ for the congruential generator of Equation (3.2).

Run length (k)	R_k	$E[R_k]$	from E_0
1	824	833.34	
2	1074	1041.66	
3	440	458.33	
4	113	131.94	
5	42	28.77	
≥ 6	7	5.95	

$\chi^2_6 = 18.10$, significant at the 2% level, using a two-tail test. Thus here the test rejects the hypothesis that the variables are random and uniform.

Before the work of Levene and Wolfowitz (1944), runs tests were incorrectly used, incorporating the standard chi-square approach. Unfortunately the algorithm by Downham (1970) omitted the $\{a_{ij}\}$ terms of Equation (6.1). That this omission could possibly result in erroneous conclusions is demonstrated by Grafton (1981), who provides a brief comparison between the correct runs test and the spectral test. Grafton (1981) provides a FORTRAN algorithm which tests 'runs down' as well as 'runs up', though the two tests are not independent. See also Section A1.2 for the IMSL routines GTRN and GTRTN. Accounts of the power of runs tests vary, and are clouded by incorrect uses of the tests. Kennedy and Gentle (1980, pp. 171-173) provide the theory for the case of runs up and down.

6.5 Repeating empirical tests

One might expect a poor generator to fail empirical tests, but a failure of an empirical test need not necessarily indicate a poor generator. Conversely, a poor generator can pass empirical tests, and both of these instances are illustrated in the following two examples.

EXAMPLE 6.4

The frequency test was applied to the (781, 387; 1000) generator, starting the sequence with 1. The full cycle was divided into 20 consecutive groups of 50 numbers each. For any group the frequency test was satisfied, but the 20 chi-square statistics took just one of the three values, 10.0, 8.8, 7.2.

EXAMPLE 6.5

The PET generator produced the borderline 5% significance result of Example 6.2(b) under the gap test. Nine subsequent gap tests produced the insignificant statistics of:

9.49, 14.88, 6.50, 13.73, 7.80, 7.80, 4.36, 8.12, 7.80

A similar 'unlucky start' is found with the frequency test applied to the decimal digits of e (Stoneham, 1965).

These difficulties can sometimes be resolved by repeating an empirical test, producing in effect a more stringent test. Chi-square values from repeating tests can be interpreted in a number of ways: a simple graphical representation can be obtained by probability (also called $Q-Q$) plots (see for example, Chernoff and Lieberman, 1956; Gerson, 1975; and Kimball, 1960), in which a sample of size n from some distribution (chi-square in our case) is ordered and plotted against the expected values of the order statistics. The expected order statistics for chi-square distributions are provided by Wilk *et al.* (1962), and two illustrations are provided by the following two examples.

EXAMPLE 6.6

The RANDU generator, $(65\ 539, 0; 2^{31})$, resulted in the probability plot shown in Fig. 6.2 for 30 applications of the 'runs up' test, each applied to a sequence of 5000 numbers.

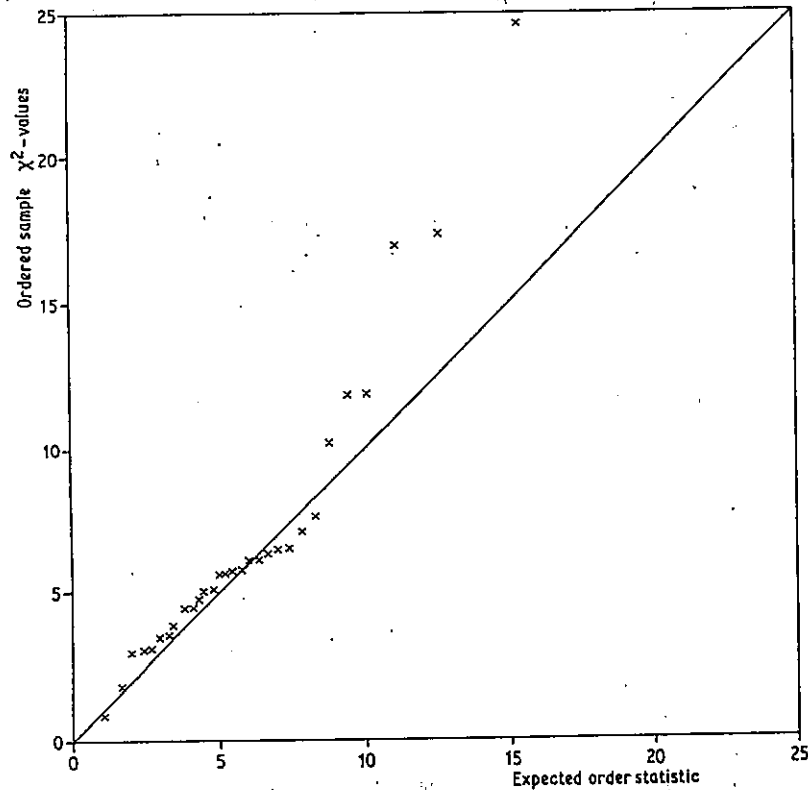


Figure 6.2 A probability plot of 30 test-statistics resulting from the 'runs up' test applied to the RANDU generator. The ordered sample is plotted against the expected order statistics for a sample of size 30 from a χ_6^2 distribution.

EXAMPLE 6.7

Stoneham (1965) made a study of the first 60 000 decimal digits of e . The results of 12 applications of the poker test are illustrated in Fig. 6.3, each test being applied to a block of 5000 consecutive digits. Some of the detail is presented in Exercise 6.15.

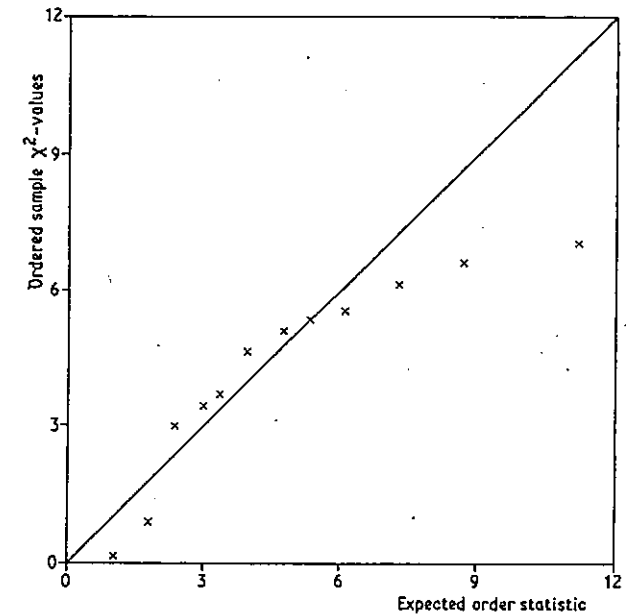


Figure 6.3 A probability plot of 12 test-statistics resulting from the poker test applied to decimal digits of e . The ordered sample is plotted against the expected order statistics for a sample of size 12 from a χ_5^2 distribution.

Note, however, that Wilk *et al.* (1962) remark that it is difficult to interpret such plots for fewer than 20 points, reaching their conclusion after applying the plots to simulated data.

Whether or not these plots indicate significant departures from the appropriate chi-square distribution can also be judged by means of a further chi-square test, if the sample size permits, as demonstrated in the next example.

EXAMPLE 6.8

The Cugini *et al.* (1980) program for the frequency test applies the test to 1050 numbers in the $(0, 1)$ range, categorizing them according to 21 equal-length intervals. The test is then repeated 60 times, and the resulting chi-square statistics are themselves categorized according to the percentile range into

which the values fall. Applying this test to the PET generator produced the following result:

% range	Actual count	Expected count
0-1	4	0.6
1-5	0	2.4
5-10	2	3
10-25	10	9
25-50	18	15
50-75	15	15
75-90	7	9
90-95	2	3
95-99	2	2.4
99-100	0	0.6
	60	60

Combining the first three and the last three rows allows us to perform a chi-square test, now on 5 degrees of freedom, to this table. We obtain the value of $\chi^2_5 = 1.82$, which is not significant at the 10% level, and so these numbers pass this empirical test.

An alternative approach is to use the Kolmogorov-Smirnov test, which is described by Hoel (1954, p. 345) and Knuth, 1981 (pp. 45-52) who provides some interesting comparisons of power between the chi-square and Kolmogorov-Smirnov tests. Categorization of the individual chi-square values is unnecessary for the Kolmogorov-Smirnov test, and when applied to the sample of size 12 illustrated in Fig. 6.3, the test does not reveal a significant departure from the expected χ^2_5 distribution at the 5% level. While the same is true for the sample of size 30 illustrated in Fig. 6.2, in that case the result is significant at the 6% level.

6.6 Tests of non-uniform random variables

We have already seen, in the last example, an illustration of the chi-square test being used to test a non-uniform (in this case also chi-square) random variable. The same approach may be used, with suitable combining of categories when necessary, for any distribution; see Exercise 6.19 for an illustration. The Kolmogorov-Smirnov test may also be used for any distribution, and, as above, does not require categorization. We shall now briefly consider some particular tests for non-uniform random variables.

6.6.1 Normal variables

Wold (1954) obtained standard normal random variables, to 2 decimal places, by transforming the digits of Kendall and Babbington-Smith (1939); the digits were initially grouped to correspond to $U(0, 1)$ variates and then the table-look-up method of Section 5.2 was used (see Example 5.4). Except for normal variables in the tails of the distribution, for the two-place accuracy needed, just four decimal place accuracy was necessary for the $U(0, 1)$ variates. The resulting table had 25 000 items, which were tested as a whole, as well as in groups of 500 and 5000. Four tests were employed:

- The numbers in a group were summed, and the result referred to the appropriate normal distribution (see Exercise 2.8(a)).
- The squares of the numbers in a group were summed, and the result referred to the appropriate chi-square distribution (see Exercise 2.5). As the group sizes are ≥ 500 , we can use the approximation that if X has a χ^2_ν distribution, $(\sqrt{2X} - \sqrt{2\nu - 1})$ is approximately $N(0, 1)$ (see Exercise 6.24).
- From the solution to Exercise 6.4 we see that if R is the range from a random sample of size n from an $N(0, 1)$ distribution, then

$$\Pr(R \leq r) = n \int_{-\infty}^{\infty} (\Phi(x+r) - \Phi(x))^{n-1} \phi(x) dx \quad (6.2)$$

and thus the ranges of such samples of size n can be obtained and compared with what one would expect, using a chi-square test. The distribution of (6.2) is tabulated in Pearson and Hartley (1970, 178-183).

- A runs test was applied to the runs of signs only of the sequence of numbers.

As with the Kendall and Babbington-Smith (1939a) tables, a note was appended to each set of numbers that failed any test.

Other tests for normality are discussed by Pearson *et al.* (1977) and Wetherill *et al.* (1984, chapter 8). One of these tests, by Shapiro and Wilk (1965), tests for departures from linearity in the appropriate probability plot.

*6.6.2 Multivariate normal variables

If (X_1, X_2) has the bivariate normal density function of Section 2.15, then the derived univariate statistic,

$$D^2 = \frac{1}{(1-\rho^2)} \left\{ \left(\frac{X_1 - \mu_1}{\sigma_1} \right)^2 - 2\rho \frac{(X_1 - \mu_1)(X_2 - \mu_2)}{\sigma_1 \sigma_2} + \left(\frac{X_2 - \mu_2}{\sigma_2} \right)^2 \right\} \quad (6.3)$$

has a χ^2_2 distribution (i.e. exponential of mean 2); see Exercise 6.5. Healy (1968a) proposed using sample values of D^2 and comparing them with the chi-

square distribution they would have if (X_1, X_2) is indeed bivariate normal. Once again a graphical examination can be made with the aid of a probability plot, the expected order statistics in a sample of size n from a χ^2_2 distribution being:

$$\frac{2}{n}, \left\{ \frac{2}{n} + \frac{2}{(n-1)} \right\}, \left\{ \frac{2}{n} + \frac{2}{(n-1)} + \frac{2}{(n-2)} \right\}, \dots, \left\{ \frac{2}{n} + \frac{2}{(n-1)} + \dots + \frac{2}{1} \right\}$$

(see Cox and Lewis, 1966, p. 27). In practice the parameters of (6.3) have to be estimated from the data, and there is discussion of this in Barnett and Lewis (1978, pp. 212–215 and 226). This approach can also be extended for general multivariate normal distributions. For additional tests see Mardia (1980), Gnanadesikan (1977, p. 161) and Royston (1983).

6.6.3 Exponential and Poisson variables

A random sample from any exponential density may be illustrated by using the order-statistics of the last section after a preliminary scaling (see Exercise 2.2). Tests for exponential random variables were used by Barnett (1965), who, in contrast to Wold, transformed pseudo-random variables, using a multiplicative congruential generator with $m = 2^{27}$, and the transformation of Equation (5.5). Five tests were then applied to the resulting numbers, including an extension of the test of Cox (1955) for detecting the presence of first-order serial correlation in a sequence of exponential variables. Barnett (1965) also generated and tested χ^2_1 variates by squaring $N(0, 1)$ variables derived by the Box-Muller method of Section 4.2.1. In connection with some of his tests, Barnett was confident that only the right-hand tail of the chi-square distribution need be used for the test critical region.

The mean and variance of Poisson random variables are equal, and the index of dispersion test makes use of this result to provide a particular test for the Poisson distribution. If (x_1, \dots, x_n) is a random sample from a Poisson distribution of parameter λ , then

$$\frac{\sum_{i=1}^n (x_i - \bar{x})^2}{\bar{x}}$$

is, approximately, a realization of a χ^2_{n-1} random variable, where

$$\bar{x} = \frac{\sum_{i=1}^n x_i}{n}$$

See for example ABC, p. 314.

6.7 Discussion

The very first tabulation, by Tippett (1927), of random digits did not include an account of any systematic testing. By contrast, the testing of random variables has now become a standard procedure, and a description of a variety of computerized algorithms which may be used is given in Section A1.2. A suite of test programs such as that of Cugini *et al.* (1980) indicates the kind of compromise that may be reached in the choice of a suitable subset of empirical tests.

The need to match tests of numbers to the intended application for those numbers is graphically illustrated by the insignificant result of the Kolmogorov-Smirnov test of Example 6.6. The RANDU generator that is tested here has very poor properties when one considers successive triples of numbers, as explained by Exercise 3.25, yet the generator does not fail at the 5% level the repeated runs test of Example 6.6.

The RANDU generator failed the extension of the serial test to three dimensions when this test was applied by Dieter and Ahrens (1974, p. A8): each time the test was applied the resulting chi-square test statistics were roughly 100 standard deviations from the expected chi-square mean for the test. However, only one (a poker test) of the many other empirical tests applied indicated that the generator had poor properties. Caution is clearly the key word. The possible problems with pseudo-random numbers are evident, and true random numbers could be biased in unexpected ways. For instance, Kendall and Babbington-Smith (1938) selected digits from the London telephone directory and found appreciably fewer 5's and 9's than one would expect (see Exercise 6.8). They attributed this to the high acoustic confusion between five and nine (airline pilots use 'fife' and 'niner' respectively), and telephone engineers selecting numbers to try to reduce this effect (for related work, see Morgan *et al.*, 1973, and Exercise 9.10).

Neave (1973) showed that when certain pseudo-random variables were transformed by the Box-Muller transformation of Section 4.2.1, the resulting variables displayed unusual characteristics. For instance, observed frequencies in the intervals $(-\infty, -3.3)$ and $(3.6, \infty)$ were zero, compared with expectations (for 10^6 generated values) of 483 and 159 respectively. However, it has been pointed out subsequently (see, e.g., Golder and Settle, 1976) that this effect is mainly due to the $(131, 0; 2^{35})$ generator used, which was considered earlier in Example 6.3 (see also Exercise 6.25). Atkinson (1980) in fact uses the Box-Muller transformation combined with a test of normal random variables as a test of the underlying generator.

6.8 Exercises and complements

6.1 Compare the bounds on the first-order serial correlation given by Equation (3.3) for a mixed congruential generator with empirical first-

order serial correlations obtained for a sequence of length 1000, for the following generators:

$$\begin{aligned} &(781, 387; 10^3) \\ &(6941, 2433; 10^4) \\ &(5^{17}, 0; 2^{42}) \end{aligned}$$

Note that an additional test of random numbers is provided by comparing empirical serial correlations with their expectation for a random sequence (see, e.g., Cugini *et al.*, 1980).

- *6.2 Perform the index-of-dispersion test for the Poisson distribution using the following sample statistics obtained using the PET generator and the program of Fig. 4.4

λ	n	\bar{x}	s^2
5	500	4.960	4.804
2	500	1.856	1.679
1	500	1.060	1.140
1	500	0.974	1.076
1	500	1.018	1.080
0.5	500	0.438	0.463

Here $s^2 = \sum_{i=1}^n (x_i - \bar{x})^2 / (n - 1)$.

- *6.3 Two dice were thrown 216 times, and the number of sixes at each throw were:

No. of sixes	0	1	2	Total
Frequency	130	76	10	216

Test the hypothesis that the probability of a six is $p = 1/6$.

Explain how this test would be modified if the hypothesis to be tested is that the distribution is binomial with the parameter p unknown. (Based on an Oxford A-level question, 1978).

- 6.4 Verify the formula for the distribution function of Equation (6.2), for the range of a random sample of size n from an $N(0, 1)$ distribution.
- *6.5 Use the formula of Equation (2.4) to verify that the random variable of Equation (6.3) has a χ^2_2 distribution.

- *6.6 (The coupon-collector problem applied to the digits 0-9) The probability that the full set of digits is obtained for the first time at the j th digit of a sequence is given by:

$$\Pr(j) = 10^{1-j} \sum_{v=1}^{10} (-1)^{v+1} \binom{9}{v-1} (10-v)^{j-1} \quad \text{for } j \geq 10.$$

Two different ways of proving this result are suggested below.

- (i) If the number of digits until the first occurrence of a complete set is denoted by S , then (verify) we can write

$$S = 1 + \sum_{i=2}^{10} X_i$$

where X_i has the geometric distribution of Section 2.6, with $p = ((11-i)/10)$, $2 \leq i \leq 10$.

Show that the probability generating function (see Section 2.16) of S is given by:

$$G(z) = \frac{9! z^{10}}{\prod_{i=1}^9 (10-iz)}$$

which, further, may be written as:

$$G(z) = \frac{9z^{10}}{10^9} \sum_{i=1}^9 (-1)^{9-i} \frac{i^8}{(10-iz)} \binom{8}{i-1}$$

Finally, by expanding this expression as a power series in z , verify the distributional form of S given above.

- (ii) An alternative approach uses the theory of occupancy problems, in which r balls are thrown at random into n cells, with $r \geq n$. In our case, each digit corresponds to a ball and each type of digit (0, 1, ..., etc.) is a cell.

If $u(r, n) = \Pr(\text{no cell is empty when } r \text{ balls are thrown at random into } n \text{ cells})$,

then we see that

$$u(r, 10) = \Pr(S \leq r),$$

and so $\Pr(S = r) = u(r, 10) - u(r-1, 10)$.

Use this approach, coupled with the fact that

$$\Pr(\text{no cell is empty}) = 1 - \Pr(\text{at least one is empty})$$

to obtain $\Pr(S = r)$.

NOTE (Feller, 1957, p. 59) that the median of the distribution of S is 27; $\Pr(S > 50) > 0.05$; $\Pr(S > 75) \approx 0.0037$. Note further that $u(r, n)$ may be used to solve the 'birthday problem': $n = 365$,

r = number of people in a room; if e.g., $r = 1900$; $\Pr(\text{no day is not represented as a birthday}) \approx 0.135$.

- 6.7 Greenwood (1955) obtained the following results from the coupon-collector test applied to the first 2486 digits in the decimal expansion of $e = 2.71828 \dots$ and the first 2035 digits in the decimal expansion of $\pi = 3.14159 \dots$ (reproduced by permission of the American Mathematical Society)

Number of digits to the full collection	π		e	
	Observed	Expected	Observed	Expected
10-19	13	11.604	12	14.202
20-23	13	11.720	11	14.344
24-27	9	11.491	14	14.064
28-32	5	11.480	15	14.050
33-39	13	10.195	17	12.477
40+	14	10.510	13	12.863
X^2 values:	6.436		2.826	

Verify the expected values given above and discuss the non-significance of the result for e in relation to the failure of the frequency test by these digits (see Metropolis *et al.*, 1950).

- 6.8 (i) Kendall and Babbington-Smith (1938) obtained the following distribution of 10 000 digits from the London telephone directory:

Digit	0	1	2	3	4	5	6	7	8	9	Total
Frequency	1026	1107	997	966	1075	933	1107	972	964	853	10000

Verify that the frequency test results in $\chi^2_9 = 58.582$.

- (ii) Fisher and Yates (1948) obtained the following distribution of digits obtained from suitably reading tables of logarithms:

Digit	0	1	2	3	4	5	6	7	8	9	Total
Frequency	1493	1441	1461	1552	1494	1454	1613	1491	1482	1519	15000

Verify that the frequency test results in $\chi^2_9 = 15.63$, and discuss their decision to remove at random 50 of the 6's, and then replace them

with other digits, chosen at random. For additional discussion, see Kendall and Babbington-Smith (1939b).

- 6.9 Comment on the following test statistics resulting from applying the 'runs up' test to sequences of 5000 numbers from the generators indicated:

Generator	Sequence		
	1	2	3
(131, 0; 2^{35})	9.89	2.70	18.10
(65539, 0; 2^{31})	13.16	5.59	12.70
(23, 0; $10^8 + 1$)	6.83	14.62	11.90
(3025, 0; 67 108 864)	10.87	3.53	3.75
PET-	5.16	2.26	8.20
The generator of Equation (3.1)	5.03	4.23	6.90

- 6.10 Verify that for the sequence of numbers from the (781, 387; 10^3) generator there are no runs up of length greater than 4, and discuss this result.
- 6.11 Apply tests of this chapter to the digits of Tables 3.1 and 3.2, and of Exercise 3.10. For many years the established decimal expansion for π was that of William Shanks, computed over a 20-year period to 707 decimal places. It was noted that 7 appeared only 51 times. In 1945 it was noticed that Shanks made an error on the 528th decimal, and all subsequent decimals are wrong. In the correct series the frequency of 7's is as one would expect (Gardner, 1966, p. 91).
- 6.12 Consider how you might construct a sequence of numbers which pass the frequency test, but which fail the serial, gap, poker and coupon-collector tests.
- 6.13 A test which is sometimes used (see, e.g., Cugini *et al.*, 1980) is the 'maximum-of- t ' test. Here numbers are taken in disjoint groups of size t , and the largest number is recorded for each group. The resulting maxima are then compared with the expected distribution.

$$\text{If } M = \max(U_1, U_2, \dots, U_n)$$

where the $\{U_i\}$ are independent, identically distributed $U(0, 1)$ random variables, show that M has the density function

$$f_M(x) = nx^{n-1} \quad \text{for } 0 \leq x \leq 1.$$

What is the distribution of M^n ?

†6.14 A further test is the permutation test, in which, again, numbers are taken in groups of size t . Here the ordering of the numbers is recorded, and the empirical distribution of the orderings compared with expectation, which allots a probability of $1/t!$ for independent uniformly distributed numbers. (The possibility of tied values is not considered.) The following results were obtained for the PET generator and the case $t = 4$.

Permutation	Number of cases	Permutation	Number of cases
1	9	13	11
2	17	14	12
3	16	15	10
4	9	16	7
5	6	17	9
6	6	18	13
7	10	19	9
8	12	20	12
9	10	21	7
10	10	22	8
11	8	23	10
12	11	24	8

Assess the significance of these results using a chi-square test.

*6.15 (Stoneham, 1965) The detail of six of the poker test results presented in Example 6.7 and Fig. 6.3 is given below:

Block	Hands					
	All different	One pair	Two pairs	One triple	One triple and one pair	4 or 5 of the same kind
1	316	506	98	70	5	5
2	307	499	108	80	6	0
3	317	503	90	72	13	5
4	299	511	114	58	12	6
5	299	498	99	84	18	2
6	307	503	111	67	8	4
Theoretical frequencies for random digits	302.4	504	108	72	9	4.6

Verify the theoretical frequencies and the resulting chi-square values.

Block	1	2	3	4	5	6
χ^2_5	3.42	6.62	5.53	4.61	5.32	7.05

6.16 Invent a test of your own for uniform random numbers.

6.17 Investigate and test the random number generators that are available to you. This can be quite revealing. Miller (1977a, 1977b) and Bremner (1981), have revealed errors in Texas hand-calculator multiplicative congruential generators. Furthermore, Bremner has pointed out that the RND function available in the University of Kent implementation of BASIC is (3025, 0; 67 108 864), and not (3125, 0; 67 108 864), as intended, and for which test results were available! (See Pike and Hill, 1965). Nevertheless, the (3025, 0; 67 108 864) generator passes the empirical tests of Cugini *et al.* (1980). (See also Exercise 6.27.)

6.18 (Cooper, 1976) The Box-Muller method involves computing the functions, log, square-root, sin and cos, for each pair of normal random variables generated. If (as in Barnett, 1965) the aim is to simulate χ^2_4 variables, show how the number of functions computed can be reduced.

6.19 Use a chi-square test to compare the p.d.f. and histogram of Fig. 2.5. The frequencies illustrated by the histogram are:

2, 4, 8, 18, 19, 12, 14, 14, 5, 2, 2

Repeat this approach for other appropriate figures from Chapter 2, reading the frequencies from the histograms/bar-charts.

6.20 Wold defined the P -value for each test as the two-tail probability of being as, or more, extreme as the resulting value of the test-statistic. Thus, for example, the sum of the first 500 numbers was $S = 159.97$, $\Phi(159.97/\sqrt{5000}) = 0.9882$, and $P = 2(1 - 0.9882) = 0.0237$. In addition to the tests already described, he wrote:

'For each type of test, the distribution of P -values obtained from the 50 page sets has been compared with the expected distribution, which is rectangular over the interval (0; 1). On the whole, the agreement with the expected distribution is good. The deviations have been tested by the χ^2 method, grouping the distribution in 10 equal intervals. The P -values obtained for the 4 tests are 49.4, 13.7, 29.0 and 91.1% respectively. The agreement was also tested by the method of Kolmogoroff, mentioned above, a method not involving grouping, with the results $P = 15.5, 42.6, 26.6$ and 98.9%.

Discuss his approach and conclusions (cf. Section 6.5).

6.21 The 30 test statistics illustrated in Fig. 6.2 are given below:

0.84	1.82	2.92	3.01	3.06	3.43	3.51	3.84	4.43	4.45
4.74	5.02	5.09	5.61	5.64	5.73	5.77	6.11	6.12	6.33
6.47	6.52	7.09	7.62	10.20	11.84	11.88	16.93	17.32	24.59

Use a chi-square test to assess whether these values come from a χ^2_6 distribution. The Kolmogorov-Smirnov test of Example 6.6, applied to these data, was made with the aid of the NAG FORTRAN routine GO1BCF, which evaluates the right-hand tail areas, assuming these values form a random sample from χ^2_6 ; and GO8CAF, using the option: null = 1, which performs a Kolmogorov-Smirnov test of whether these tail areas are uniform (cf. Exercise 6.20). Tail areas for chi-square densities are also given in Pearson and Hartley (1972, p. 160). For computational formulae see Kennedy and Gentle (1980, Section 5.7).

6.22 Use the results of Exercise 2.8 to construct particular tests for exponential and Poisson variables. How might you make use of the result of Exercise 4.17?

*6.23 Use the results of Exercise 4.14 to simulate bivariate normal random variables, and test them using the approach of Section 6.6.2

*6.24 In Section 6.6.1 we used the result:

If X has a χ^2_ν distribution, for large ν , then

$N = \sqrt{2X} - \sqrt{2\nu - 1}$ is approximately $N(0, 1)$.

Why is this? (Note that the results of Section 2.12 are exact, while here we are seeking an approximate relationship.)

*6.25 Neave (1973) combined a multiplicative congruential generator with only the sine form of the Box-Muller transformation (see Section 4.2.1), obtaining

$$N = (-2 \log_e U_1)^{1/2} \sin(2\pi U_2)$$

in which $x_2 = ax_1 \pmod{m}$,

and $U_1 = x_1/m; U_2 = x_2/m$.

Show that we can write N in the form:

$$N = (-2 \log_e U)^{1/2} \sin(2\pi aU)$$

Chay *et al.* (1975) suggested using the $\{U_i\}$ from the multiplicative congruential generator in the opposite order to that above, resulting in:

$$N = (-2 \log_e U_2)^{1/2} \sin(2\pi U_1)$$

Show that $x_1 = a^*x_2 \pmod{m}$

where $aa^* = 1 \pmod{m}$

so that the 'Chay interchange' is equivalent to changing the multiplier in the generator, and keeping to the original sequence. Kronmal (1964) applied the Box-Muller transformation to pseudo-random numbers from two mixed congruential generators, one for U_1 and another for U_2 , and found that the resulting numbers passed a variety of tests.

6.26 Write computer programs to perform the tests considered in this chapter.

*6.27 Conduct empirical tests of the (25 173, 13 849; 2^{16}) generator. T. Hopkins has pointed out that this generator, proposed by Grogono (1980), performs badly on the spectral test. The choice of multiplier here appears to be particularly unfortunate, as literally hundreds of alternative multipliers give rise to a much better result on the spectral test. Consider, for example, (13 453, 13 849; 2^{16}).

6.28 What will the result be if the frequency test is applied to the entire cycle of a full-period mixed congruential generator? What are the implications of this result?

*6.29 Given a sequence of pseudo-random numbers, how would you test whether or not a cycle was present?

VARIANCE REDUCTION AND INTEGRAL ESTIMATION

7.1 Introduction

In the preceding chapters we have seen how to generate uniform random variables, and we have considered ways of transforming these to produce other common random variables. Having tested our random variables, we are well prepared for using them in a simulation exercise. However, before pressing on in a bull-at-a-gate fashion it is worth while first of all considering whether the efficiency of the approach to be adopted could be increased. Andrews (1976) writes:

'In a recent Monte Carlo study of a regression problem the computing cost was about £250. The cost of generating the required 160 000 Gaussian [normal] deviates was 50p, a negligible amount relative to the total cost. I have found that variance reduction methods often apply. As these affect sample size they affect the remaining £249.50. Modest gains in efficiency result in large savings; very efficient methods can often be found.'

Thus variance reduction is a way of improving value for money, and it can result in much greater savings than those involved in just changing from one algorithm to another for generating variates. As we shall see, there are many different variance-reduction techniques, and a ready way of illustrating these techniques arises in the context of integral estimation using random numbers. The above quotation used the term 'Monte Carlo'; this is now frequently employed as a more evocative synonym for simulation when random variables are employed. 'Monte Carlo' frequently also has an implied connotation of some variance-reduction method having been used. (See, for example, Cox and Smith, 1961, p. 128; Gross and Harris, 1974, p. 383; and Schruben and Margolin, 1978, for related discussion.) It is an item of folklore that this term was introduced as a code-word for secret simulation work in connection with the atomic bomb during the Second World War (Rubinstein, 1981, p. 11).

The basic idea of variance reduction is contained in the following example.

EXAMPLE 7.1 Buffon's cross

The Buffon needle experiment has already been described in Exercise 1.2. If a thin needle of length l is thrown at random on to an infinite horizontal table with parallel lines a distance $d \geq l$ apart, then the probability that the needle will cross a line is given by $2l/\pi d$. This probability may be estimated by the proportion of crossings in an experiment consisting of a number of successive throws of a needle, and knowledge of l and d then enables us to estimate π . From the data of Exercise 1.2, we see that π is not very precisely estimated in this way (cf. the precision of Exercise 3.10), even for as many as 960 throws of the needle. Soldiers recovering from wounds sustained during the American Civil War had the time, and apparently also the interest (Hammersley and Handscomb, 1964, p. 7), for multiple repeats of the needle experiment, but present-day experimenters are unlikely to be so patient.

One way to speed the process up is to throw more than one needle each time, and then the picking up of the needles is facilitated if the needles are joined together. In its simplest form, this is accomplished by fusing two needles of equal length at right-angles at their centres, to form a cross. If Z denotes the total number of lines intersected from a single throw of the cross, we can write $Z = X + Y$, where X and Y separately denote the number of crossings of each of the two needles. The distribution of X , and equivalently Y , is unaffected by the presence of the other needle, and so $\mathcal{E}[X] = \mathcal{E}[Y] = 2l/(\pi d)$, and $\mathcal{E}[Z] = 4l/(\pi d)$. The best approach is to take $l = d$ (see Exercise 1.2), and let us, in this case set $\theta = 2/\pi$. X and Y are simple binomial random variables and so (see Table 2.1), $\text{Var}(X) = \text{Var}(Y) = \theta(1-\theta)$.

It can be shown that the distribution of Z is given by:

$$\begin{cases} \Pr(Z=0) = 1 - \frac{2\sqrt{2}}{\pi}; & \Pr(Z=1) = 4(\sqrt{2}-1)/\pi; \\ \Pr(Z=2) = 4(1-1/\sqrt{2})/\pi \end{cases}$$

This enables us to evaluate $\text{Var}(Z) = \text{Var}(X) + \text{Var}(Y) + 2\text{Cov}(X, Y)$, yielding, ultimately,

$$\text{Cov}(X, Y) = 2(\pi(2 - \sqrt{2}) - 2)/\pi^2 \approx -0.0324$$

reflecting the fact that the needles are fixed together, and X and Y are not independent: $\text{Corr}(X, Y) = -0.14$.

In the original Buffon experiment, $\text{Var}(\hat{\theta}) \approx 0.2313/n$, where n denotes the number of throws of the needle. In the case of the cross, from one throw, $\hat{\theta} = \frac{1}{4}(X+Y)$, and so, because of the term $\frac{1}{2}$ we immediately have a reduction in $\text{Var}(\hat{\theta})$, for

$$\text{Var}(\hat{\theta}) = \frac{1}{4}(\text{Var}(X) + \text{Var}(Y) + 2\text{Cov}(X, Y)) = \frac{1}{2}\text{Var}(X) + \frac{1}{2}\text{Cov}(X, Y)$$

and $\text{Cov}(X, Y) < 0$

Thus fixing the two needles together has a utility over and above the added ease of collecting the needles. For n throws of the cross, $\text{Var}(\hat{\theta}) \approx 0.0995/n$. So we see that using a cross, rather than a single needle, is a variance-reduction technique; it results in greater precision, i.e. an estimator of smaller variance. Against this gain must be offset the labour of correctly fixing the needles to form a cross (though this is more easily done by etching a cross on a clear perspex disc), and the computation of the new theory. These losses occur once only, and would clearly be worth while if a very large experiment were envisaged. There is no reason why further gains should not be obtained from the use of more than two fused needles, and Kendall and Moran (1963, p. 72) provide the result for the case of a star shape; see Hammersley and Morton (1956) for details. In the case of a star, further additional labour (small for a cross) is involved in counting the number of crossed lines. The converse to changing the needle is changing the grid, and Perlman and Wichura (1975) provide the theory for the case of square and triangular grids. Further discussion and elaboration are to be found in Mosteller (1965, pp. 86–88) and Ramaley (1969), as well as Exercises 7.1–7.4.

The extended example above illustrates the basic features of a variance-reduction method, and we shall encounter these features again in the next section. Of course the above example is artificial in that we already know π , which permits a simple evaluation of the variance reduction achieved.

A fundamental aspect of the above example, and others to follow, is the estimation of a parameter θ by an estimator $\hat{\theta}$, with

$$E[\hat{\theta}] = \theta \quad \text{and} \quad \text{Var}(\hat{\theta}) \propto n^{-1}.$$

In both the needle and the cross cases, $\hat{\theta}$ is proportional to a sum of random variables, and hence for large n (and typically n is large in such experiments), central limit theorems apply, so that $\hat{\theta} \approx N(\theta, \kappa/n)$, for appropriate κ . Thus as well as simply producing the estimate $\hat{\theta}$, we can also obtain approximate confidence intervals for θ ; for example, a 95% confidence interval is $(\hat{\theta} \pm 1.96 \kappa^{1/2}/n^{1/2})$, when the normal approximation is valid. The width of this interval is $\propto n^{-1/2}$, so that, for instance, to halve an interval width one has to quadruple the number of observations. Because of this feature it is clearly desirable to employ a variance-reduction technique that results in as small a value for κ as possible.

7.2 Integral estimation

A definite integral, such as $\Phi(x)$, which cannot be explicitly evaluated, can be obtained by a variety of numerical methods. Some of these are described by Conte and de Boor (1972), and algorithms are available for programmable hand-calculators, as well as within computer subroutine libraries such as

NAG. For numerical evaluation of integrals in a small number of dimensions one would therefore be unlikely to use simulation. However, simulation methods can be viable for high-dimensional integration, say in the dimensional range 6–12 (Davis and Rabinowitz, 1975, p. 314). In this section we refer solely to simple one-dimensional integrals, as they provide a convenient vehicle for illustrating some basic methods of variance reduction. [It is in any case interesting to see how random numbers may be used to evaluate deterministic integrals. In the following we shall again consider estimation of π , but now through the representation:

$$\frac{\pi}{4} = \int_0^1 \sqrt{1-x^2} dx \quad (7.1)$$

each side of (7.1) being the area of a quadrant of a circle of radius unity.]

7.2.1 Hit-or-miss Monte Carlo

The integral of (7.1) is the area of a quadrant of the circle, radius 1 and centre 0. If that quadrant is enclosed by a unit square, and points thrown independently at random on to the square, then the proportion R/n of n points thrown that land within the quadrant can be used as an estimate of the probability, $\pi/4$, of any point landing within the quadrant; see Fig. 7.1(a). Thus $4R/n$ can be used as an estimate of π . Now R is a random variable with a $B(n, \pi/4)$ distribution, with $\text{Var}(R) = n\frac{\pi}{4}(1-\frac{\pi}{4})$ so that $\text{Var}(4R/n) = 16 \text{Var}(R)/n^2 = \pi(4-\pi)/n \approx 2.697/n$.

$R = \text{succ}$
 $\frac{R}{n} = \frac{\pi}{4}$
 $B(n, \frac{\pi}{4})$
Binomial

7.2.2 Crude Monte Carlo

As $\frac{\pi}{4} = \int_0^1 \sqrt{1-x^2} dx$, we can write

$\pi/4 = E[\sqrt{1-U^2}]$, where U is a $U(0, 1)$ random variable, and so if we take a random sample, U_1, U_2, \dots, U_n , we can estimate $\pi/4$ by:

$$I = \frac{1}{n} \sum_{i=1}^n \sqrt{1-U_i^2}$$

This approach is termed 'crude' Monte Carlo.

Clearly, $\text{Var}(I) = n^{-1} \text{Var}(\sqrt{1-U^2})$

$$= n^{-1} \left(\int_0^1 (1-x^2) dx - \left(\int_0^1 \sqrt{1-x^2} dx \right)^2 \right)$$

$$= n^{-1} \left(\frac{2}{3} - \frac{\pi^2}{16} \right)$$

$$\approx 0.0498/n$$

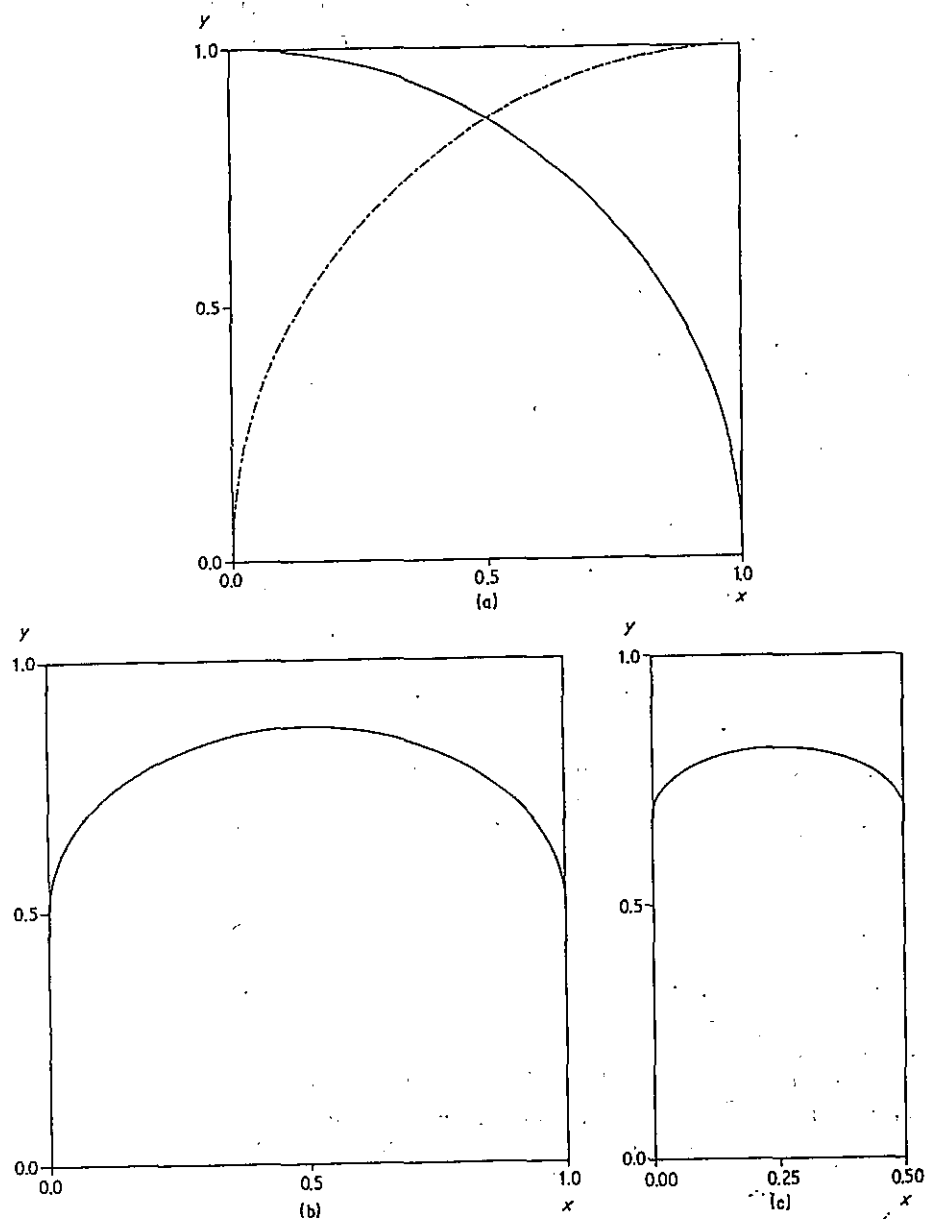


Figure 7.1 A graphical demonstration of variance reduction

(a) — $y = \sqrt{1-x^2}$; - - - $y = \sqrt{1-(1-x)^2}$

(b) $y = \frac{1}{2} \{ \sqrt{1-x^2} + \sqrt{1-(1-x)^2} \}$

(c) $y = \frac{1}{4} \{ \sqrt{1-x^2} + \sqrt{1-(1-x)^2} + \sqrt{1-(\frac{1}{2}-x)^2} + \sqrt{1-(\frac{1}{2}+x)^2} \}$

The area under the curves of (a) and (b) is $\pi/4$; the area under the curve of (c) is $\pi/8$.

To construct a point at random within a unit square, we only need to take a point with Cartesian co-ordinates (U_1, U_2) , where U_1 and U_2 are independent $U(0, 1)$ variables. In order to compare the 'hit-or-miss' and crude Monte Carlo approaches to estimating π we can take $2n$ $U(0, 1)$ variables in each case, resulting in the respective variances of estimators of π :

$$\frac{2.697}{n} \quad \text{and} \quad 0.0498 \times 16/2n = 0.398/n$$

So we see that the variance in the hit-or-miss case is roughly seven times larger than in the crude case, indicating that crude Monte Carlo is much more efficient.

7.2.3 Using an antithetic variate

Let $H = \frac{1}{2} \{ \sqrt{1-U^2} + \sqrt{1-(1-U)^2} \}$,

where U is $U(0, 1)$, $(1-U)$ is the 'antithetic' variate to U . As both U and $(1-U)$ are $U(0, 1)$ random variables,

$\mathcal{E}[H] = \pi/4$, but now

$$\begin{aligned} \text{Var}(H) &= \frac{1}{4} \{ \text{Var}(\sqrt{1-U^2}) + \text{Var}(\sqrt{1-(1-U)^2}) \\ &\quad + 2 \text{Cov}(\sqrt{1-U^2}, \sqrt{1-(1-U)^2}) \} \\ &= \frac{1}{2} \{ \text{Var}(\sqrt{1-U^2}) + \text{Cov}(\sqrt{1-U^2}, \sqrt{1-(1-U)^2}) \} \\ &= \frac{1}{2} \left(\frac{2}{3} - \frac{\pi^2}{16} \right) + \frac{1}{2} \mathcal{E} \left[\sqrt{((U+1)U(U-1)(U-2))} - \frac{\pi^2}{16} \right] \end{aligned}$$

It can be shown that

$$\begin{aligned} \mathcal{E} \left[\sqrt{((U+1)U(U-1)(U-2))} \right] &= \frac{\pi}{4} \left\{ \frac{71}{96} - 6 \sum_{k=2}^{\infty} \frac{(2k-3)!(2k-1)!(12)^{-2k}}{(k-2)!(k-1)!k!(k+1)!} \right\} \\ &\approx 0.5806 \end{aligned}$$

leading to:

$$\text{Var}(H) = 0.0052.$$

Thus if $2n$ $U(0, 1)$ variates were used to estimate π using this antithetic approach, the resulting estimator would have variance $0.042/n$. The crude estimator variance is just over nine times larger than this, while the hit-or-miss estimator variance is roughly 64 times larger. In real terms this means that to obtain the same precision using the hit-or-miss and antithetic approaches, we need 64 times as many uniform variates in the hit-or-miss approach. Of course there may be losses in the different types of arithmetic involved between these two different approaches. We commented on this aspect in our comparison of the Buffon needle and cross, and we can now see that the second needle of the cross produced an antithetic variate, resulting in the negative correlation between X and Y in Section 7.1. The idea of using antithetic variates was formally introduced by Hammersley and Morton (1956), who explained the idea through the example of Buffon's needle.

*7.2.4 Reducing variability

The reduction in variability obtained by the use of an antithetic variate as above is simply seen from a comparison of the curves of Fig. 7.1(a) and 7.1(b): the ranges of the y -values are, respectively, 1, $(\sqrt{3}-1)/2$, while the areas under the curves are each $\pi/4$. We can clearly reduce variability even further by using the curve of Fig. 7.1(c), enabling us to estimate π using:

$$H = \left\{ \sqrt{(1-U^2)} + \sqrt{(1-(1-U)^2)} + \sqrt{(1-(\frac{1}{2}-U)^2)} + \sqrt{(1-(\frac{1}{2}+U)^2)} \right\} \quad (7.2)$$

where now U is $U(0, 0.5)$. This process can be continued without end, rather like the testing of random numbers. Again a compromise has to be reached, in this case between variance reduction and increase in computation. For more discussion of this approach, see Morton (1957) and Shreider (1964, p. 53).

The variability in $y = \sqrt{(1-x^2)}$ can be reduced in a number of additional ways. For instance, we can write

$$y = \{1-x^2\} + \{\sqrt{(1-x^2)} - (1-x^2)\} \quad \text{for } 0 \leq x \leq 1 \quad (7.3)$$

as suggested in Simulation I (1976, p. 41). In (7.3), of course, both the components of y can be integrated explicitly, but if one knows how to integrate $\{1-x^2\}$ and not $\sqrt{(1-x^2)}$, then the decomposition of (7.3) replaces the variability of $\sqrt{(1-x^2)}$ by the smaller variability of $\{\sqrt{(1-x^2)} - (1-x^2)\}$. A decomposition of y can also be obtained without introducing a new function, simply by splitting up the range of x , and evaluating the integral as the sum of the integrals over the separate parts of the x -range. This is called *stratified sampling*, and is familiar to students of sampling theory (see Barnett, 1974, p. 78). For illustration, suppose the function to be integrated is $y = f(x)$, over the range $(0, 1)$, (see Fig. 7.2).

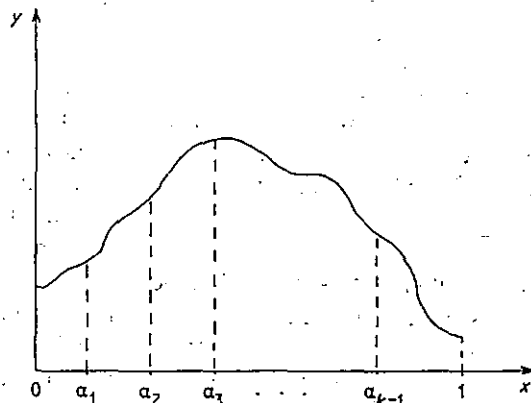


Figure 7.2 Stratified sampling for Monte Carlo integral estimation.

We shall break the range of integration into k pieces, of length $(\alpha_j - \alpha_{j-1})$, for $1 \leq j \leq k$, with $0 = \alpha_0 < \alpha_1 < \dots < \alpha_k = 1$. Clearly, the variability of y within each piece is less than the variability of y over the full range. Estimation of the sub-integrals may be done in each case by, for example, crude Monte Carlo. If we use n_j $U(0, 1)$ variates for the j th interval, then we can estimate $\theta = \int_0^1 f(x) dx$ by:

$$\hat{\theta} = \sum_{j=1}^k \sum_{i=1}^{n_j} \frac{(\alpha_j - \alpha_{j-1})}{n_j} f(\alpha_{j-1} + (\alpha_j - \alpha_{j-1})U_{ij})$$

in which the U_{ij} are independent $U(0, 1)$ random variables. Thus

$$Y_{ij} = \alpha_{j-1} + (\alpha_j - \alpha_{j-1})U_{ij} \quad \text{is } U(\alpha_{j-1}, \alpha_j)$$

as required for crude Monte Carlo estimation within the j th interval. The terms $(\alpha_j - \alpha_{j-1})$ are weights which are needed to ensure that $\hat{\theta}$ is unbiased.

We see that

$$\begin{aligned} E[\hat{\theta}] &= \sum_{j=1}^k \sum_{i=1}^{n_j} \frac{(\alpha_j - \alpha_{j-1})}{n_j} \int_0^1 f(\alpha_{j-1} + (\alpha_j - \alpha_{j-1})x) dx \\ &= \sum_{j=1}^k \left(\frac{\alpha_j - \alpha_{j-1}}{n_j} \right) \int_{\alpha_{j-1}}^{\alpha_j} \frac{f(x) dx}{(\alpha_j - \alpha_{j-1})} \left(\sum_{i=1}^{n_j} 1 \right) \\ &= \sum_{j=1}^k \int_{\alpha_{j-1}}^{\alpha_j} f(x) dx = \int_0^1 f(x) dx = \theta \end{aligned}$$

In order to examine the precision of this approach we need the variance of $\hat{\theta}$:

$$\text{Var}(\hat{\theta}) = \sum_{j=1}^k \sum_{i=1}^{n_j} \frac{(\alpha_j - \alpha_{j-1})^2}{n_j^2} \text{Var}(f(\alpha_{j-1} + (\alpha_j - \alpha_{j-1})U_{ij}))$$

which leads readily to:

$$\text{Var}(\hat{\theta}) = \sum_{j=1}^k \frac{1}{n_j} \left\{ (\alpha_j - \alpha_{j-1}) \int_{\alpha_{j-1}}^{\alpha_j} f^2(x) dx - \left(\int_{\alpha_{j-1}}^{\alpha_j} f(x) dx \right)^2 \right\} \quad (7.4)$$

In using stratified sampling, one has to choose k , $\{\alpha_j\}$, $\{n_j\}$. Increasing k , the number of pieces, or strata, is likely to increase precision, but results in more arithmetic labour, and as before, a compromise is usually reached. For given k and $\{\alpha_j\}$, one can try to choose the $\{n_j\}$ to minimize the variance of (7.4).

We can write

$$\text{Var}(\hat{\theta}) = \sum_{j=1}^k \frac{a_j}{n_j}$$

say, and we want to choose the $\{n_j\}$ to minimize $\text{Var}(\hat{\theta})$, subject to a restriction such as $\sum_{j=1}^k n_j = n$, for fixed n . We can incorporate the constraint by

introducing a Lagrange multiplier, λ , and then minimizing the Lagrangian:

$$L = \sum_{j=1}^k \frac{a_j}{n_j} - \lambda \left(n - \sum_{j=1}^k n_j \right)$$

Stationary values are obtained by setting

$$\frac{\partial L}{\partial n_j} = 0 \quad \text{for } 1 \leq j \leq k,$$

$$\text{i.e. } a_j = \lambda n_j^2, \quad \text{for } 1 \leq j \leq k.$$

Standard theory (see Exercise 7.6) verifies that this stationary value is indeed a minimum, obtained by selecting the

$$n_j \propto a_j^{1/2} = (\alpha_j - \alpha_{j-1}) \sqrt{\text{Var}(f(\alpha_{j-1} + (\alpha_j - \alpha_{j-1})U_{ij}))} \quad (7.5)$$

Unfortunately, as we can see from (7.4), a_j involves the very integral we are seeking, and so is unknown. However, the message of (7.5) is clear, suggesting that the larger strata, and strata with more variable function values, should receive relatively more variates, as one would expect. Thus one could, as a rough rule of thumb, choose the $\{\alpha_j\}$ to correspond, as closely as possible, to parts of the curve with a constant range of y -values, and then allot the $\{n_j\}$ in proportion to $\{(\alpha_j - \alpha_{j-1})\}$. Alternatively, one could conduct a preliminary experiment to estimate the unknown variances in (7.5), and then use those estimates in deciding upon the $\{n_j\}$ for a full, subsequent investigation.

*7.2.5 Importance sampling

In stratified sampling, proportions n_j/n of n $U(0, 1)$ variables are transformed to the range (α_{j-1}, α_j) . This is not dissimilar from selecting the U_{ij} variates which go to form $\hat{\theta}$ from the composition density function:

$$\Psi(x) = \sum_{j=1}^k \left(\frac{n_j}{n} \right) \eta_j(x) \quad (7.6)$$

$$\text{in which } \eta_j(x) = \begin{cases} 1/(\alpha_j - \alpha_{j-1}) & \text{for } \alpha_{j-1} \leq x < \alpha_j \\ 0 & \text{otherwise} \end{cases} \quad \text{for } 1 \leq j \leq k.$$

The continuous analogue of (7.6) is found in *importance sampling*, so called because, as with (7.6), $f(x)$ is evaluated at the important parts of the range more frequently than otherwise. Continuing with the above illustration, let us further suppose $f(x) > 0$ for $0 \leq x \leq 1$, and also that $g(x)$ is a probability density function over this range.

$$\begin{aligned} \theta &= \int_0^1 f(x) dx = \int_0^1 \frac{f(x)}{g(x)} g(x) dx \\ &= \mathcal{E}[f(X)/g(X)], \text{ when } X \text{ has probability density function } g(x). \end{aligned}$$

If (X_1, \dots, X_n) constitutes a random sample from $g(x)$, then we can estimate θ by:

$$\hat{\theta} = \frac{1}{n} \sum_{i=1}^n \frac{f(X_i)}{g(X_i)}$$

which has variance given by

$$\begin{aligned} \text{Var}(\hat{\theta}) &= \frac{1}{n} \left\{ \int_0^1 \frac{f^2(x)}{g(x)} dx - \theta^2 \right\} \\ &= 0 \text{ if } g(x) = \theta^{-1} f(x) \end{aligned} \quad (7.7)$$

which would clearly be a good form to adopt for $g(x)$. Unfortunately, this entails knowledge of the unknown θ before $g(x)$ can be specified. However, if $g(x)$ is of roughly the same shape as $f(x)$ then (7.7) will hold approximately, and so we would expect the $\hat{\theta}$ that results to have small variance.

EXAMPLE 7.2 An illustration of importance sampling

$$\text{Evaluation of } \Phi(x) = \int_{-\infty}^x \frac{e^{-y^2/2}}{\sqrt{2\pi}} dy = \int_{-\infty}^x \phi(y) dy$$

We have seen already in Example 5.4 how this distribution function may be used in simulation, and we know that it is not possible to evaluate the integral explicitly. A density curve of similar shape to $\phi(y)$ is the logistic:

$$f(y) = \frac{\pi \exp(-\pi y/\sqrt{3})}{\sqrt{3}(1 + \exp(-\pi y/\sqrt{3}))^2}$$

with mean 0 and variance 1, already encountered in Section 5.7.

$$\Phi(x) = \int_{-\infty}^x \frac{k\phi(y) f(y)}{f(y) k} dy$$

where k is chosen so that $f(y)k^{-1}$ is a density function over the range $(-\infty, \infty)$.

$$\text{Thus } f(y)k^{-1} = \frac{\pi \exp(-\pi y/\sqrt{3})(1 + \exp(-\pi x/\sqrt{3}))}{\sqrt{3}(1 + \exp(-\pi y/\sqrt{3}))^2} \quad (7.8)$$

and if Y is a random variable with the density function of (7.8) then,

$$\Phi(x) = (1 + \exp(-\pi x/\sqrt{3}))^{-1} \mathcal{E}[\phi(Y)/f(Y)]$$

We can therefore estimate $\Phi(x)$ by:

$$\hat{\theta} = \frac{1}{n} (1 + \exp(-\pi x/\sqrt{3}))^{-1} \sum_{i=1}^n \phi(Y_i)/f(Y_i)$$

where $\{Y_i, 1 \leq i \leq n\}$ is a random sample from the density of Equation (7.8).

conveniently simulated by means of the inversion method of Section 5.2 as follows. If U is a $U(0, 1)$ random variable,

$$\text{set } U = F(Y) = (1 + \exp(-\pi x/\sqrt{3})) / (1 + \exp(-\pi Y/\sqrt{3}))$$

then we seek $Y = F^{-1}(U)$, resulting in:

$$Y = -\frac{\sqrt{3}}{\pi} \log_e \{ (1 + \exp(-\pi x/\sqrt{3})) U^{-1} - 1 \}$$

A BASIC program to evaluate $\Phi(x)$ in this way is given in Fig. 7.3 for a selection of x -values, and results from using this program are shown in Table 7.1.

```

10 RANDOMIZE
20 REM PROGRAM TO CALCULATE PHI(X)
30 REM USING IMPORTANCE SAMPLING
40 INPUT N
50 LET P1 = 1.813799364
60 LET X = -2.5
70 FOR K = 1 TO 4
80 LET X = X+.5
90 LET S = 0
100 FOR I = 1 TO N
110 LET R = (1+EXP(-X*P1))/RND
120 LET Y = -(LOG(R-1))/P1
130 LET P2 = (EXP(-Y*Y/2))/2.506628275
140 LET Q = (P2*(1+EXP(-Y*P1))-2)*EXP(Y*P1)
150 LET S = S+Q
160 NEXT I
170 LET S = S/N
180 LET S = S/(P1*(1+EXP(-X*P1)))
190 PRINT X,S,N
200 NEXT K
210 END

```

Figure 7.3 A BASIC program to evaluate $\Phi(x)$ using importance sampling. Note that $\pi/\sqrt{3} \approx 1.813799364$, and $\sqrt{2\pi} \approx 2.506628275$.

An application of importance sampling in queueing theory is provided by Evans *et al.* (1965).

Table 7.1

x	Estimated $\Phi(x)$			Actual $\Phi(x)$ (from tables) to 4 d.p.
	$n = 100$	$n = 1000$	$n = 5000$	
-2.0	0.0222	0.0229	0.0229	0.0227
-1.5	0.0652	0.0681	0.0666	0.0668
-1.0	0.1592	0.1599	0.1584	0.1587
-0.5	0.3082	0.3090	0.3081	0.3085

We shall not here consider $\text{Var}(\hat{\theta})$ for this example, but see the solution to Exercise 7.7.

7.3 Further variance-reduction ideas

7.3.1 Control variates

With antithetic variates, negative correlation was used to reduce variance. One can also use positive (or negative) correlation with some additional, *control* variate. As with stratified sampling, comparisons can be made here with elements of sampling theory.

Suppose X is being used to estimate a parameter θ , and $\mathcal{E}[X] = \theta$. If Z is a random variable with known expectation μ , then for any positive constant c , we can write

$$Y = X - c(Z - \mu)$$

Thus Y , like X , is an unbiased estimator of θ , as $\mathcal{E}[Y] = \mathcal{E}[X] = \theta$. Whether or not Y is a better estimator of θ than X depends on the relationship between X and Z . Now $\text{Var}(Y) = \text{Var}(X) + c^2 \text{Var}(Z) - 2c \text{Cov}(X, Z)$, and so if $\text{Cov}(X, Z) > c \text{Var}(Z)/2$, then $\text{Var}(Y)$ will be less than $\text{Var}(X)$, indicating that Y is the better estimator. The maximum variance reduction is obtained when $c = \text{Cov}(X, Z)/\text{Var}(Z)$, and while $\text{Cov}(X, Z)$ (and possibly also $\text{Var}(Z)$) may not be known, it could be estimated by means of a pilot investigation. However, many investigators have simply taken $c = \pm 1$ as appropriate.

We shall see an example of the use of a control variate in Section 9.4.2. More than one control variate may be used, and a variety of different approaches have been employed to obtain the desired correlation between the variate of interest, X , and the control variate, Z . See, for example, Law and Kelton (1982, Section 11.4). Improvements in the use of control variates are considered by Cheng and Feast (1980). A recent application is provided by Rothery (1982), in the context of estimating the power of a non-parametric test, and an illustration from queueing theory is given in the following example.

EXAMPLE 7.3 (Barnett, 1965, p. XVII): Machine interference

A mechanic services n machines which break down from time to time. We suppose that machines break down independently of one another, and that for any machine, breakdowns are events in a Poisson process of rate λ . We suppose also that the time taken to repair any machine is a constant, μ . The interference arises if queues of broken-down machines form. This process can be solved analytically, but it was presented by Barnett as an illustration of the use of a control variate. It is clearly simple to simulate the process, and to estimate the 'machine availability', S , over a time period of length t , by

$$\hat{S} = \frac{\text{total cumulative running time for all machines}}{nt}$$

As the control variate, Barnett used the estimate, \hat{L} , of $1/\lambda$, given by

$$\hat{L} = \mu \times \frac{\text{total cumulative running time for all machines}}{\text{total cumulative repair time for all machines}}$$

It was estimated empirically that the correlation between \hat{S} and \hat{L} was $\approx +0.95$ for a variety of values of n , t and the product $\lambda\mu$. Thus S was estimated by

$$\hat{S}_1 = \hat{S} - c \left(\hat{L} - \frac{1}{\lambda} \right)$$

and c was chosen as indicated above for maximum variance reduction, using estimates of second-order moments obtained from a pilot study. It was estimated that $\text{Var}(\hat{S})/\text{Var}(\hat{S}_1) \approx 9.87$. (Further discussion of this example is given in Exercises 7.22 and 7.23.)

The standard approach for estimating $\theta = \mathcal{E}[X]$ is by forming

$$\hat{\theta} = \frac{\sum_{i=1}^n X_i}{n}$$

where $\{X_i, 1 \leq i \leq n\}$ forms a random sample from the distribution of X . This is completely analogous to the averaging approaches used in the previous examples in integral estimation, which is to be expected, since here θ is a mean value which, for continuous random variables, can be written as an integral, and vice versa. As was pointed out in Section 7.2, integrals of low dimensionality are probably best evaluated by a numerical method which does not involve simulation. However, while one can certainly think of the estimation of a mean of a random variable in terms of evaluating an integral, in this case the integrand is itself almost certainly going to be a function of the (unknown) mean, and so simulation methods are then appropriate.

When a model is to be simulated under different conditions, and comparisons made between the different simulations, then the variation between the simulations can be reduced by using common random numbers in the different simulations. This is a very popular method of variance reduction and, as with many uses of control variates; it relies on an induced positive correlation for its effect. We shall return to the use of common random numbers in Chapter 9. A good example, involving the comparison of alternative queueing mechanisms, is given by Law and Kelton (1982, p. 352).

*7.3.2 Using simple conditioning

The principle here is best illustrated by means of an example.

EXAMPLE 7.4 (Simon, 1976)

Suppose we want to estimate the mean value θ of a random variable X , which has the beta $B_e(W, W^2 + 1)$ distribution, where W itself is a random variable, with a Poisson distribution of known mean, η . The obvious approach is to simulate n X -values and simply average them. However, this involves simulation from Poisson and beta distributions; and an alternative approach is as follows.

We know, from Section 2.11, that

$$\mathcal{E}[X|W = w] = w/(w^2 + w + 1)$$

Furthermore,

$$\sum_{w=0}^{\infty} \mathcal{E}[X|W = w] \frac{e^{-\eta} \eta^w}{w!} = \theta$$

(here we are using a property of conditional expectation—see Grimmett and Stirzaker, 1982, p. 44).

So we may estimate θ by

$$\hat{\theta} = \frac{1}{n} \sum_{i=1}^n w_i / (w_i^2 + w_i + 1)$$

where the $\{w_i, 1 \leq i \leq n\}$ form a random sample from the Poisson distribution, parameter μ ; a procedure which does not, in fact, involve simulating X . Thus this approach certainly saves labour. Discussion of how the variance of the above estimator may be further reduced is given in Exercise 7.20. In a different context, Lavenberg and Welch (1979) use conditioning to reduce variance in a particular queueing network, and their example is reproduced by Law and Kelton (1982, p. 364).

7.3.3 The M/M/1 queue

It is interesting to see how variance-reduction techniques that have been clearly expressed for simple procedures, such as the evaluation of one-dimensional integrals, may be employed in more complicated investigations. We shall here consider the M/M/1 queue. This model of a simple queue has already been encountered in Exercise 2.27, which also provided a BASIC program for the simulation of the queue.

We are often interested in the average customer waiting-time in a queue. The waiting time of the n th customer, from arrival at the queue until departure, W_n , may be very simply expressed as:

$$\begin{cases} W_n = (W_{n-1} - I_n + S_n) & \text{if } W_{n-1} \geq I_n \\ W_n = S_n & \text{if } W_{n-1} < I_n \end{cases} \quad (7.9)$$

where S_n is the service-time of customer n , and

I_n is the time between the arrival of the n th and $(n-1)$ th customers, for $n \geq 2$.

Note here that we take $W_1 = S_1$, i.e., the first customer arrives to find an empty queue. Figure 7.4 provides a BASIC program for simulating this queue, for which the service and inter-arrival times are both exponential, with respective parameters $\mu = 1$, $\lambda = 0.6$. We see that the average waiting-time is computed for 200 customers. The process is then repeated 100 times so as to provide an estimate of the variance of the average waiting time. The program of Fig. 7.4 provides a much simpler way of estimating average waiting-time than direct use of the program of Exercise 2.27, and we shall return to this point in Chapter 8.

```

10 REM BASIC PROGRAM TO ESTIMATE THE AVERAGE
20 WAITING TIME OF THE FIRST 200 CUSTOMERS
30 REM AT AN M/M/1 QUEUE, STARTING EMPTY, USING (7.9)
40 LET L=.6
50 LET M=1
60 RANDOMIZE
70 LET T1=0
80 LET T2=0
90 FOR J=1 TO 100
100 LET S2=0
110 LET W=0
120 FOR I=1 TO 200
130 LET U=RND
140 LET S=(-LOG(U))/M
150 LET U=RND
160 LET T=(-LOG(U))/L
170 IF W<T THEN 200
180 LET W=W+S-T
190 GOTO 210
200 LET W=S
210 LET S2=S2+W
220 NEXT I
230 LET T1=T1+(S2/200)
240 LET T2=T2+(S2/200)*2
250 NEXT J
260 LET V=(T2-(T1*T1)/100)/99
270 PRINT "VARIANCE OF AVERAGE WAITING TIME = ",V
280 PRINT "MEAN = ",T1/100
290 END

```

Figure 7.4 A BASIC program to estimate the average waiting-time of the first 200 customers at an M/M/1 queue, starting empty. The procedure is repeated 100 times. Note that in lines 140 and 160 the method of Equation (5.5) is used.

This is an example where an antithetic-variate approach could prove useful. Figure 7.5 provides another BASIC program for simulating this queue. In this case we duplicate each block of 200 customers, and in the duplicate block each original U is replaced by $(1 - U)$, with the result that long service times are replaced by short services times, and vice versa, and similarly also for inter-arrival times. Each block average therefore still estimates the same average waiting time, but the two duplicate block averages might now be expected to have a negative correlation. Table 7.2 illustrates the results of the start of a run of the program of Fig. 7.5, and we can see here the anticipated relationship developing between the two sets of W_n values. Proofs that variance reduction will occur when antithetic variates are used in this, and more general, queueing

```

10 REM ILLUSTRATION OF VARIANCE REDUCTION USING
20 REM ANTITHETIC VARIATES IN AN M/M/1 QUEUE
30 DIM R(400)
40 LET L=.8
50 LET M=1
60 LET I1=0
70 RANDOMIZE
80 LET U1=0
90 LET U2=0
100 LET T1=0
110 LET T2=0
120 LET N=50
130 FOR J=1 TO N
140 FOR I=1 TO 400
150 LET R(I)=RND
160 NEXT I
170 LET S2=0
180 LET W=0
190 LET K=0
200 FOR I2=1 TO 200
210 LET K=K+1
220 LET U=R(K)
230 LET S=(-LOG(U))/M
240 LET K=K+1
250 LET U=R(K)
260 LET T=(-LOG(U))/L
270 IF W<T THEN 300
280 LET W=W+S-T
290 GOTO 310
300 LET W=S
310 LET S2=S2+W
320 NEXT I2
330 IF I1=1 THEN 360
340 LET S5=S2/200
350 GOTO 400
360 LET S5=(S5+S2/200)/2
370 LET T1=T1+S5
380 LET T2=T2+S5*S5
390 GOTO 460
400 FOR I=1 TO 400
410 LET R(I)=1-R(I)
420 NEXT I
430 REM THIS FORMS THE ANTITHETIC VARIATES
440 LET I1=1
450 GOTO 170
460 LET I1=0
470 NEXT J
480 LET V=(T2-T1*T1/N)/(N-1)
490 PRINT "VARIANCE OF AVERAGE WAITING TIME=" ,V
500 PRINT "ESTIMATE OF MEAN WAITING TIME=" ,T1/N
510 END

```

Figure 7.5 A BASIC program to estimate the average waiting-time of the first 200 customers in an M/M/1 queue, starting empty. The procedure is based upon Equation (7.9) and uses antithetic variates, as explained in the text.

models are provided by Mitchell (1971) and others (see Kleijnen, 1974, p. 190), who also provide empirical investigations, as do Law and Kelton (1982, p. 356).

A variety of results from running the programs of Figs 7.4 and 7.5 are given in Table 7.3. We can see, by considering the results from different runs, that the estimate of efficiency gain can vary appreciably, but in all comparisons there is a gain in efficiency. Use of equations (7.9) does in fact contravene a basic rule for variance reduction, already encountered in (7.3) (see also Exercises 7.8 and

Table 7.2 An illustration of the use of Equation (7.9) to compute waiting times in an M/M/1 queue, and the effect of replacing service (S_n) and inter-arrival times (T_n) by their antithetic counterparts.

n	Main block			Antithetic block			
	S_n	T_n	W_n	n	S_n	T_n	W_n
1	1.35	—	1.35	1	0.30	—	0.30
2	0.20	0.40	1.15	2	1.70	1.34	1.70
3	0.75	1.89	0.75	3	0.64	0.22	2.12
4	0.17	0.36	0.56	4	1.88	1.42	2.58
5	0.43	0.97	0.43	5	1.05	0.60	3.03
6	1.83	0.39	1.87	6	0.18	1.34	1.23

7.20), as we shall now explain. We can write

$$W_n = Q_n + S_n \quad \text{for } n \geq 1$$

where Q_n is the time spent by the n th customer queuing before being served. Q_n and S_n are independent, and $\text{Var}(Q_n) < \text{Var}(W_n)$. Therefore in order to estimate $E[W_n]$ it is more efficient to estimate $E[Q_n]$ and then add on the known $E[S_n] = 1/\mu$. This can be seen from a comparison of Tables 7.3(a) and (b). This comparison also suggests, however, that the use of (7.9) combined with an antithetic-variate approach can increase efficiency, relative to the use of (7.10) below combined with antithetic variates. Note that

$$Q_n = \max(Q_{n-1} + S_n - I_n, 0) \quad (7.10)$$

Table 7.3 (a) Sample variance of the estimator of the mean waiting-time of the first 200 customers in an M/M/1 queue, starting empty and with $\mu = 1$. 100 replications were used in each case, with 50 matched pairs when antithetic variates were employed. In this case the waiting-times were simulated including the service-times, i.e. using Equation (7.9)

λ	Run	No variance reduction	Using antithetic variates
		0.5	1
	2	0.1426	0.0736
	3	0.2174	0.0561
		0.1646	0.0686
0.6	1	0.3102	0.1338
	2	0.4010	0.1851
	3	0.5233	0.1676
		0.4115	0.1622

(contd.)

Table 7.3 (contd.)

λ		No variance reduction	Using antithetic variates
		0.7	1
	2	5.4315	0.4734
	3	1.0977	0.3401
		2.9515	0.3523
0.8	1	2.7757	1.2451
	2	6.6679	1.6539
	3	6.7081	2.1598
		5.3839	1.6863

Corresponding average waiting-times of the first 200 customers.

λ	Run	No variance reduction	Using antithetic variates	Theoretical value in equilibrium (see Exercise 7.24)
		0.5	1	
	2	2.035	2.020	2.0
	3	2.030	1.984	
		1.985	2.001	
0.6	1	2.513	2.464	
	2	2.467	2.408	2.5
	3	2.533	2.543	
		2.504	2.472	
0.7	1	3.320	3.041	
	2	3.497	3.199	3.33
	3	3.051	3.241	
		3.289	3.160	
0.8	1	4.244	4.392	
	2	4.416	4.404	5.0
	3	5.152	4.451	
		4.604	4.416	

(b) The following results are obtained by simulating the waiting-times without the service-times, i.e. using Equation (7.10). First of all we give the sample variances, as in (a).

λ		No variance reduction	Using antithetic variates
	<i>Run</i>		
0.5	1	0.1314	0.0927
	2	0.1547	0.0902
	3	0.1225	0.0466
		<hr/>	<hr/>
		0.1362	0.0765
0.6	1	0.3228	0.2487
	2	0.6141	0.1521
	3	0.5180	0.1182
		<hr/>	<hr/>
		0.4850	0.1730
0.7	1	0.8762	0.3201
	2	1.1808	0.5234
	3	0.9866	0.6251
		<hr/>	<hr/>
		1.0145	0.4895
0.8	1	6.4527	1.3440
	2	3.2618	2.0066
	3	5.4324	1.6008
		<hr/>	<hr/>
		5.049	1.6703

Corresponding average waiting-times of the first 200 customers in an M/M/1 queue, starting empty and with $\mu = 1$, as above. Values are obtained by computing the average waiting-time, excluding service, and then adding on the known mean service-time.

λ		No variance reduction	Using antithetic variates	Theoretical values in equilibrium (see Exercise 7.24)
	<i>Run</i>			
0.5	1	2.028	2.019	2.0
	2	2.000	2.034	
	3	1.936	1.989	
		<hr/>	<hr/>	
		1.988	2.014	
0.6	1	2.354	2.533	2.5
	2	2.550	2.418	
	3	2.559	2.401	
		<hr/>	<hr/>	
		2.488	2.451	

λ		No variance reduction	Using antithetic variates	Theoretical values in equilibrium (see Exercise 7.24)
0.7	1	3.129	3.300	3.33
	2	3.134	3.165	
	3	3.198	3.282	
		<hr/>	<hr/>	
		3.154	3.249	
0.8	1	4.594	4.444	5.0
	2	4.447	4.445	
	3	4.576	4.531	
		<hr/>	<hr/>	
		4.539	4.473	

As one might expect, whether we are using Equations (7.9) or (7.10), the amount of variance reduction achieved depends on the relationship between λ and μ : if λ is appreciably smaller than μ , then the queue will frequently be empty, reducing the negative correlation. The values of λ and μ also affect the rate at which a steady-state system is reached (for the case $\lambda < \mu$ - see Exercise 7.24). Barnett's (1965) tables of exponential random variables provide values of $-\log_e(1-U)$ as well as $-\log_e U$, with just such antithetic investigation in mind (see Example 7.22).

An alternative approach to antithetic variance reduction in simple queues was applied by Page (1965), who used the following idea. Suppose we are simulating an M/M/1 queue, constructing service and inter-arrival times respectively from:

$$S = -\frac{1}{\mu} \log_e(U_1)$$

$$T = -\frac{1}{\lambda} \log_e(U_2)$$

for independent $U(0, 1)$ variables U_1 and U_2 .

A duplicate run can be made with

$$\tilde{S} = -\frac{1}{\mu} \log_e(U_2)$$

$$\tilde{T} = -\frac{1}{\lambda} \log_e(U_1)$$

In this case U_1 values giving rise to large service times in the original run will be

translated into large waiting times in the duplicate run, and vice versa. Page showed that

$$\text{Corr}((S - T), (\bar{S} - \bar{T})) = -2\rho/(1 + \rho^2) \quad \text{where } \rho = \lambda/\mu.$$

*7.3.4 A simple random walk example

In random walks we are interested in the distribution of the position of a particle which moves along a line according to probability rules. A simple example results when the particle moves between absorbing barriers at 0 and a , a being a positive integer, according to the rules specified in Fig. 7.6. Exercise 1.4 provided an example of a random walk with a reflecting barrier at 0.

The particle position can be used to describe features of more complicated processes such as the population size of a colony of bacteria; the particular example of Fig. 7.6 is often called the 'gambler's ruin' problem, as the particle position can be taken as the capital of one of two gamblers, with combined capital of a units. In the game played by the gamblers, money changes hands in single units according to the probabilities p and q , and the game ends when one of the gamblers loses all his/her capital, corresponding to the particle reaching one of the barriers. Various features of this walk are of interest, such as the values $\{d_k, 1 \leq k \leq a-1\}$, where d_k is the average number of steps to termination of this walk, when the walk starts at k .

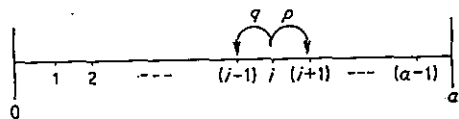


Figure 7.6 Illustration of a simple random walk. When the particle is at i (i an integer in the range $1 \leq i \leq a-1$), then, independently of the past, it moves to $(i+1)$ with probability p , and to $(i-1)$ with probability $q = (1-p)$. Once either of the barriers at 0 and a is reached, then the walk terminates.

It can be shown that the $\{d_k\}$ satisfy:

$$\begin{cases} d_k = 1 + pd_{k+1} + qd_{k-1} & \text{for } 1 \leq k \leq a-1 \\ d_0 = d_a = 0 \end{cases} \quad (7.11)$$

(see, e.g., Bailey, 1964, p. 27, and Exercise 7.30). While these equations have an explicit solution, given in Exercise 7.31, the $\{d_k\}$ can be estimated by simulation (cf. Exercise 3.29). Thus one can select a value of k , and simulate n walks, starting at k , running until absorption. d_k may then be estimated by the sample mean time to absorption. A very simple variance-reduction idea which may be used here is outlined by Barnett (1962a). If a walk starting at k passes through

some point j at a later stage, say after r steps, then if it takes n steps for the original walk to end, we also have, from this walk, an example of a walk taking $(n-r)$ steps to absorption, starting from j . Thus a single walk starting from any k can provide information on mean times to absorption for walks starting from points other than k . Clearly by this method the mean-time estimators for different values of k will not be independent. For discussion of this see Barnett (1962a), who used this approach for a two-dimensional random walk without an explicit solution; and Morgan and Robertson (1980), who considered an intractable one-dimensional problem (see Exercise 7.32).

7.4 Discussion

The aim of this chapter has been to underline the importance of variance reduction, and to introduce some of the methods that are used. Further methods and illustrations will be encountered later. Quite apart from its importance, variance reduction is attractive because of the extra information that can often be squeezed out of single random variables, this process frequently requiring a 'flash of insight', in Barnett's (1976) words. Because of the dramatic gain in value that can result, variance-reduction techniques are sometimes also termed 'swindling' (see Simon, 1976, and Schruben and Margolin, 1978, p. 524). Of course, this idea of obtaining as much value as possible from a single random variable has already been encountered, for instance in Exercise 4.2, and Example 5.5. We can also note the analogies between the rejection method of Section 5.3, and importance sampling and hit-or-miss Monte Carlo, as well as between the composition method of Section 5.4, and stratified sampling and the method of extracting an easier integral, in Section 7.2.4.

Much more detail of variance reduction is provided by Law and Kelton (1982, chapter 11), and Kleijnen (1974, chapter 3). Frequently it is necessary to run a pilot study in order to assess the possible value of a variance-reduction technique, for in complicated systems theoretical justification for employing such a technique is usually not possible. Indeed, it is unfortunately the case that in some applications variances have inadvertently been increased from using a 'reduction' approach. Cheng (1982) points out the importance of high negative correlation when antithetic variates are used, and suggests a modified procedure which has been applied successfully to a variety of models.

We saw in Section 7.1 that in many applications simulation estimators of parameters are expressed as sums of independent random variables. In these and related cases it is a simple matter to estimate variances of estimators, which are vital for the interpretation of estimates. In Section 7.2.2 the variance of the estimator involved the parameter that was being estimated. In that case, for illustration, the known parameter value was used in calculating the variance,

while in practice the variance itself would only be an estimate. Knowledge of the answer (π) has undoubtedly also affected the reporting of experiments involving Buffon's needle, as well as the decision of when to stop. As Mantel (1953) points out, Lazzerini's experiment, conducted in 1901, produced $\hat{\pi} = 3.1415929$ after 3408 throws, but ending the experiment one throw sooner or later inevitably loses half the decimal place accuracy. When one is estimating waiting-times in queues, one is averaging dependent random variables, which complicates variance estimation. A number of possible approaches for such cases are described and compared by Moran (1975), and we shall return to this topic in Chapter 8.

Additional reductions in variance may be obtained by the judicious combination of different methods (see Exercise 7.23 and Schruben and Margolin, 1978), though here again one must proceed with caution, as Kleijnen (1974, Section III.8) has shown. 'Proceed with care' is therefore clearly the watchword for variance reduction, as it was with the use of pseudo-random numbers. However, as with the use of pseudo-random numbers, the benefits from using an appropriate variance-reduction technique can be substantial. Finally, we may note that common random variables and antithetic variates are variance-reduction techniques of general applicability, in so far as the same approach is adopted, whatever the problem. In contrast, methods such as importance sampling, stratified sampling, and the use of control variates all have to be individually tailored to particular problems.

7.5 Exercises and complements

(a) On Buffon's needle

- 7.1 What is the mean number of lines crossed if $l > d$? For discussion of this case; see Mosteller (1965, p. 88) and Mantel (1953).
- *7.2 (Gani, 1980) Suppose the centre of the needle lands at a distance x from a line, and that the needle makes an angle θ with the direction of the lines. Map out the sample space for (x, θ) , and by identifying the subset of the sample space corresponding to the needle crossing a line, show that, for $l \leq d$, $\Pr(\text{needle crosses a line}) = 2l/\pi d$. When $l > d$, show that this probability must be corrected by the amount

$$\frac{2}{\pi} \cos^{-1}(d/l) - \frac{2l}{\pi d} \sqrt{(1-d^2/l^2)}.$$

- *7.3 (Perlman and Wichura, 1975) The case of a single needle thrown on to a double grid. Here we have grids, A and B, say, each of parallel lines a distance d apart, the grids being at right angles to each other. This problem was originally studied by Laplace. Let $r = d/l$, and let $p_{AB} = \Pr(\text{needle crosses an A-line and a B-line})$, $p_{\bar{A}\bar{B}} = \Pr(\text{needle crosses an$

A-line but not a B-line), etc. Show that

$$p_{AB} = \frac{r^2}{\pi}$$

$$p_{A\bar{B}} = p_{\bar{A}B} = \frac{2r}{\pi} - \frac{r^2}{\pi}$$

$$p_{\bar{A}\bar{B}} = 1 - \frac{4r}{\pi} + \frac{r^2}{\pi}$$

Separate evaluation of these probabilities may be used to estimate π , in different ways, and which one to use is an intriguing question. If in n throws of the needle there are $n_{\bar{A}\bar{B}}$, $n_{\bar{A}B}$, n_{AB} and n_{AB} throws in the four possible categories, then (verify)

$$\frac{n_{AB}}{n} \text{ is an estimator of } \frac{r^2}{\pi}$$

$$\frac{n_{\bar{A}\bar{B}} + n_{\bar{A}B} + 2n_{AB}}{n} \text{ is an estimator of } \frac{4r}{\pi}$$

$$\frac{n - n_{\bar{A}\bar{B}}}{n} \text{ is an estimator of } \frac{4r - r^2}{\pi}$$

If $r = 1$, Perlman and Wichura show that the variances of the resulting estimators are, respectively, $5.63/n$, $1.76/n$, $0.466/n$.

- *7.4 (Continuation) The following data were collected from class experiments by E. E. Bassett:

	n	$n_{\bar{A}\bar{B}}$	$n_{\bar{A}B}$	n_{AB}	n_{AB}
experiment 1	400	16	112	125	147
experiment 2	990	64	315	304	307

Use these data and the estimators of the last exercise to provide a variety of estimates of π .

Further data are provided by Kahan (1961), who describes practical problems such as the blunting of the needle with use, and Gnedenko (1976, pp. 36–39), who also considers the throwing of a convex contour. Historical background is found in Holgate (1981), who conjectures on how Buffon obtained his solution. Mantel (1953) obtains an estimator of π from the estimation of a variance, rather than a mean.

- *7.5 (Holgate, 1981) Another problem studied by Buffon was the 'Jeu du franc-carreau': a circular coin of radius b is thrown on to a horizontal

square grid of side $2a$. Show that if $b/a = (1 - 2^{-0.5})$ then the coin is as likely as not to land totally within a square.

(b) Integral estimation

- *7.6 Show that the stationary value of the Lagrangian.

$$L = \sum_{j=1}^k \frac{a_j}{n_j} - \lambda \left(n - \sum_{j=1}^k n_j \right)$$

given by: $n_j \propto a_j^{1/2}$ is a minimum.

- *7.7 When the computer program of Fig. 7.3 is run for values of $x = 0.5, 1.0, 1.5$ and 2.0 , the following values result:

x	Estimated $\Phi(x)$			$\Phi(x)$ to 4 d.p.
	n = 100	n = 1000	n = 5000	
0.5	0.6999	0.6905	0.6898	0.6915
1.0	0.8477	0.8405	0.8423	0.8413
1.5	0.9253	0.9386	0.9337	0.9332
2.0	0.9867	0.9822	0.9761	0.9773

We obtain better accuracy with the results of Table 7.1. Use the argument of Section 7.2.4 to explain why we might expect this.

- 7.8 Hammersley and Handscomb (1964, p. 51) define the relative efficiency of two Monte Carlo methods for estimating a parameter θ as follows: The efficiency of method 2 relative to method 1 is:

$$(n_1 \sigma_1^2) / (n_2 \sigma_2^2)$$

where method i takes n_i units of time, and has variance σ_i^2 , $i = 1, 2$. Write BASIC programs to estimate the integral:

$$I = \int_0^1 e^{-x^2} dx$$

by hit-or-miss, crude and antithetic variate Monte Carlo methods, and compare the efficiencies of these three methods by using a timing facility. Suggest, and investigate, a simple preliminary variance-reduction procedure. Investigations of variance reduction when

$I = \int_0^1 g(x) dx$ are given by Rubinstein (1981, pp. 135-138).

- 7.9 Write a BASIC program to estimate the integral of Exercise 7.8 using a stratification of four equal pieces, and 40 sample points. How should you distribute the sample points?

- 7.10 Explain how the use of stratification and antithetic variates may be combined in integral estimation.
- *7.11 Verify that $\int_0^1 \sqrt{\{(x+1)x(x-1)(x-2)\}} dx \approx 0.5806$.
- 7.12 Given the two strata, $(0, \sqrt{3}/2)$, $(\sqrt{3}/2, 1)$, for evaluating $\int_0^1 \sqrt{1-x^2} dx$, how would you allot the sampling points?
- *7.13 In crude Monte Carlo estimation of $\int_0^1 \sqrt{1-x^2} dx$, how large must n be in order that a 95% confidence interval for the resulting estimator of π has width v ? Evaluate such an n for $v = 0.01, 0.1, 0.5$.
- *7.14 Daley (1974) discusses the computation of integrals of bivariate and trivariate normal density functions. Describe variance-reduction techniques which may be employed in the evaluation of such integrals using simulation. For related discussion, see Simulation I (1976, Section 13.8.3) and Davis and Rabinowitz (1975, Section 5.9).
- 7.15 Repeat Exercise 7.8, using the pseudo-random number generator of Equation (3.1).

(c) General variance reduction

- 7.16 Show that the maximum variance reduction in Section 7.3.1 is obtained when $c = \text{Cov}(X, Z) / \text{Var}(Z)$.
- 7.17 (Kleijnen, 1974, p. 254) Suppose one is generating pseudo-random uniform variables from the $(a, 0; m)$ generator, with seed x_0 . Show that the corresponding antithetic variates result from using $(m - x_0)$ as the seed.
- 7.18 Suppose one wants to estimate $\theta = \text{Var}(X)$, and $X = U + V$, when U, V are independent random variables, and $\text{Var}(U)$ is known. Clearly here a simulation should be done to estimate $\text{Var}(V) < \text{Var}(X)$. Use this result to estimate $\text{Var}(M)$, where M is the median of a sample of size n from a $N(0, 1)$ distribution. You may assume (see Simon, 1976) that \bar{X} and $(M - \bar{X})$ are independent, where \bar{X} denotes the sample mean.
- 7.19 (Continuation) Conduct an experiment to estimate the extent of the variance reduction in Exercise 7.18.
- 7.20 (Simon, 1976).
- (i) Verify that $\left(\frac{W}{W^2 + W + 1} \right) = \frac{1}{(W+1)} - \frac{1}{(W+1)(W^2 + W + 1)}$.
- (ii) If W has the Poisson distribution of Example 7.4, show that $E[1/(W+1)] = (1 - e^{-\eta})/\eta$.

(iii) Show that

$$\hat{\theta} = \left(\frac{1 - e^{-\eta}}{\eta} \right) - \frac{1}{n} \sum_{i=1}^n \{(W_i + 1)(W_i^2 + W_i + 1)\}^{-1}$$

is an unbiased estimator of θ , and that $\text{Var}(\hat{\theta}) < \text{Var}(\hat{\theta}')$.

(d) Queues

*7.21 Investigate the use of the mean service-time as a control variate for the mean waiting-time in an M/M/1 queue.

7.22 For any simulation giving rise to the estimate \hat{S} in the machine-interference study of Example 7.3 we can construct an antithetic run, replacing each $U(0, 1)$ variate U in the first simulation by $(1 - U)$ in the second. If we denote the second estimator of S by \hat{S}' , then a further estimator of S is:

$$\hat{S}_2 = \frac{1}{2}(\hat{S} + \hat{S}')$$

Barnett (1965) found empirically that the correlation between \hat{S} and \hat{S}' was ≈ -0.64 , a high negative value, as one might expect. Estimate the efficiency gained (see Exercise 7.8) from using this antithetic-variate approach (cf. Fig. 7.5).

7.23 (Continuation) Barnett (1965) considered the further estimator of S :

$$\hat{S}_3 = \frac{1}{2}\{(\hat{S} + \hat{S}') - k(\hat{L} + \hat{L}' - 2/\lambda)\}$$

where \hat{L}' is the estimator of $1/\lambda$ from the antithetic run. Discuss this approach, which combines the uses of control and antithetic variates. Show how k should be chosen to maximize the efficiency gain, and compare the resulting gain in efficiency with that obtained from using control variates and antithetic variates separately.

7.24 In an M/M/1 queue, when $\lambda < \mu$, then after a period since the start of the queue, the queue is said to be 'in equilibrium', or to have reached the 'steady state'. The distribution of this period depends on λ , μ and the initial queue size. In equilibrium the queue size Q has the geometric distribution

$$\text{Pr}(Q = k) = \rho(1 - \rho)^k \quad \text{for } k \geq 0$$

where $\rho = \lambda/\mu$, and is called the 'traffic intensity'. Use this result to show that the customer waiting-time in equilibrium (including service time) has the exponential density: $(\mu - \lambda)e^{-(\lambda - \mu)x}$, and hence check the theoretical equilibrium mean values of Table 7.3. Further, comment on the disparities between the values obtained by simulation and the theoretical equilibrium mean values. For related discussion, see Rubinstein (1981, p. 213) and Law and Kelton (1982, p. 283).

Unfortunately, it is the cases when ρ is near 1, for $\rho < 1$, that are often of practical importance, but also the most difficult to investigate using simulation.

7.25 Exponential distributions are, as we have seen, often used to model inter-arrival and service-times in queues. Miss A. Kenward obtained the data given below during a third-year undergraduate project at the University of Kent. Illustrate these data by means of a histogram, and use a chi-square test to assess whether, in this case, the assumption of exponential distributions is satisfactory (cf. Exercise 2.26).

The following data were collected from the sub-post office in Ashford, Kent, between 9.00 a.m. and 1.00 p.m. on a Saturday in December, 1981.

Inter-arrivals

Time in seconds	0-10	10-20	20-30	30-40	40-50	50-60	60-70	70-80	80-90	90-100
No. of arrivals	179	108	79	37	32	21	10	13	8	4
Time in Seconds	100-110	110-120	120-130	130-140	140-150	150-160	160-170			

No. of arrivals	5	1	3	2	1	0	2
-----------------	---	---	---	---	---	---	---

Service times

Time in minutes	0-0.5	0.5-1	1-1.5	1.5-2	2-2.5	2.5-3	3-3.5	3.5-4
No. of customers	63	32	21	10	7	6	0	2
Time in minutes	4-4.5	4.5-5	5-7	7-7.5	7.5-8			

No. of customers	0	1	0	1	1
------------------	---	---	---	---	---

*7.26 (Gaver and Thompson, 1973, p. 594) Sometimes service in a queue takes a variety of forms, performed sequentially. For example, if one has two types of service: payment for goods (taking time T_1), followed by packing of goods (taking time T_2), then the service time $S = T_1 + T_2$. It is an interesting exercise to estimate $\mathcal{E}[S]$ by simulation, using antithetic variates. In an obvious notation, this would result in:

$$\hat{S} = \frac{1}{2n} \sum_{i=1}^n (T_{1i} + T_{2i} + T'_{1i} + T'_{2i}),$$

in which T'_{ji} is an antithetic variate to T_{ji} , $j = 1, 2$, $1 \leq i \leq n$. If T_1 and T_2 are independent, exponential variables, with density e^{-x} , then show that

the usual approach of taking, for example, $T'_{1i} = \log_e(1-U)$, where $T_{1i} = \log_e U$, results in:

$$\text{Var}(\hat{S}) = \frac{1}{n} \left\{ 1 + \int_0^1 \log_e x \log_e(1-x) dx \right\} = \frac{1}{n} \left(2 - \frac{\pi}{6} \right)^2 \approx 0.36/n.$$

Compare this value with that which results from a usual averaging procedure. Of course in this simple example the distribution of S is known to be $\Gamma(2, 1)$ (see Section 2.10). However, we have here the simplest example of a *network*, and for a discussion of more complicated networks see Gaver and Thompson (1973, p. 595), Rubinstein (1981, pp. 151–153) and Kelly (1979).

- 7.27 Investigate further the findings of Table 7.3 by means of a more extensive simulation. Validate your conclusions by also using the generator of Equation (3.1).
- 7.28 Ashcroft (1950) provides an explicit solution to the machine-interference problem with constant service-time, while Cox and Smith (1961, pp. 91–109) and Feller (1957, pp. 416–420) provide the theory and extensions for the case of service-times with an exponential distribution. Discuss how you would simulate such a model. Bunday and Mack (1973) consider the complication of a mechanic who patrols the machines in a particular order.
- 7.29 (Page, 1965) In the simulation of Fig. 7.5, let D_n and D'_n be defined by:

$$D_n = S_n - I_n$$

$$D'_n = S'_n - I'_n$$

Show that $\text{Corr}(D, D') = -0.645$ (cf. Exercise 7.26).

(e) Gambler's ruin

- 7.30 From a consideration of the first step taken by the particle in the gambler's ruin problem of Section 7.3.4, verify the relationships of Equation (7.11).
- *7.31 Show that the solution of Equation (7.11) is given by:

(i) the case $p \neq q$:

$$d_k = \frac{k}{(q-p)} - \frac{a}{(q-p)} \frac{(1-(q/p)^k)}{(1-(q/p)^a)} \quad 0 \leq k \leq a.$$

(ii) the case $p = q = \frac{1}{2}$:

$$d_k = k(a-k) \quad 0 \leq k \leq a.$$

- *7.32 Write a BASIC program to simulate the gambler's ruin problem of Section 7.3.4, employing the variance-reduction technique of that section, and compare estimated values of $\{d_k\}$ with the theoretical values given in the last exercise.