Time Series Analysis

Nonstationary and Noninvertible Distribution Theory

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Chapter 6 Numerical Integration

We discuss and demonstrate how to invert numerically the c.f.'s to obtain the distribution functions and the probability densities of statistics presented so far. It should be emphasized that any computer package for integration cannot do the job properly if the integrand contains the square root of a complex-valued function, like the c.f.'s we have dealt with. We present a Fortran program for this purpose.

As an integration method we use Simpson's rule, which proves to be successful for most cases. There are, however, some cases where the integrand is oscillating and converges to 0 rather slowly. For such cases Euler's transformation of slowly convergent alternating series is employed to accelerate the convergence of integration based on Simpson's rule. Various graphs and Fortran programs are presented for demonstration purposes. We also discuss the saddlepoint method for computing approximate distribution functions and percent points.

6.1. Introduction

This chapter is concerned with computing numerically the distribution functions and the probability densities of statistics which are quadratic plus linear or bilinear functionals of the Brownian motion. This necessarily entails inverting the c.f.'s of those statistics. As we have seen, the c.f. is usually expressed as the square root of a complex-valued function, which any computer cannot compute properly. We first need to devise an algorithm for evaluating the square root correctly.

After obtaining the correct c.f., we proceed to examine the behavior of the integrand to find an effective interval of the integral together with a suitable method for integration. We shall find Simpson's rule successful in most cases, but we shall also use Euler's transformation of slowly convergent alternating series for cases where the integrand is oscillating and converges to 0 rather slowly. Since it is usually the case that the difficulty arises not in the computation of distribution functions, but in that of probability densities, we shall also consider a practical method for computing the latter on the basis of the former.

The next section deals with statistics that take only nonnegative values with well behaved c.f.'s. The procedure for computing distribution functions and probability densities is explained in detail with Fortran programs which can be executed by a desktop computer. The oscillating case is discussed in Section 3, where Euler's transformation is introduced to make the computation more accurate and efficient. Section 4 deals with a general case where statistics take both positive and negative values. A practical method is considered here for computing probability densities. Section 5 discusses how to obtain percent points of distribution functions. A Fortran program is also presented to demonstrate the methodology. The last section describes briefly the saddlepoint method for computing approximate distribution functions and percent points.

6.2. Numerical integration : the nonnegative case

Let S be a nonnegative statistic, for which we would like to compute the distribution function and the probability density. Lévy's inversion theorem for nonnegative random variables tells us that

$$
\begin{aligned}
(6.1) \qquad F(x) &= P(S \le x) \\
&= \frac{1}{\pi}\int_0^\infty \mathrm{Re}\left[\frac{1-e^{-i\theta x}}{i\theta}\,\phi(\theta)\right] d\theta\,,
\end{aligned}
$$

where $\phi(\theta)$ is the c.f. of S.

If $F(x)$ is differentiable, we have the probability density of S given by

$$
\begin{aligned}
(6.2) \qquad f(x) &= \frac{dF(x)}{dx} \\
&= \frac{1}{\pi}\int_0^\infty \mathrm{Re}\left[e^{-i\theta x}\phi(\theta)\right] d\theta\,.
\end{aligned}
$$

Our purpose here is to devise an efficient method for numerical integration associated with (6.1) and (6.2). We can recognize, from the computational point of view, that the distribution function is handled more easily than the probability density since the integrand in the former converges to 0 more rapidly.

There is, however, a problem prior to numerical integration in (6.1) and (6.2). The c.f. $\phi(\theta)$ is usually the square root of a complex-valued function, which any computer cannot evaluate properly. As an example let us consider

$$
(6.3) \qquad \phi_1(\theta) = \left(\frac{\sin\sqrt{2i\theta}}{\sqrt{2i\theta}}\right)^{-\frac{1}{2}}\,,
$$

which is the c.f. of a nonnegative statistic defined by

$$
\begin{aligned}
S_1 &= \int_0^1 \left(w(t) - \int_0^1 w(s)ds\right)^2 dt \\
&= \int_0^1\int_0^1 [\,\min(s,t) - st\,]\, dw(s)dw(t)\,.
\end{aligned}
$$

Figure 6.1 draws the computer-generated graph of $\phi_1(\theta)$, $\tilde{\phi}_1(\theta)$, say. It is seen that there is a discontinuity point in $\mathrm{Im}(\tilde{\phi}_1(\theta))$ at around $\theta = 15$ where $\mathrm{Re}(\tilde{\phi}_1(\theta)) = 0$. Since $\phi_1(\theta)$ is continuous for all θ, this graph is not correct, although $|\tilde{\phi}_1(\theta)| = |\phi_1(\theta)|$. If we had replaced $\tilde{\phi}_1(\theta)$ by $-\tilde{\phi}_1(\theta)$ at the discontinuity point and the successive points, we would have obtained a correct graph.

Figure 6.1

To obtain the correct c.f., Nabeya and Tanaka (1988) used the following algorithm. We start computing a c.f. $\phi(\theta)$ at $\theta = \theta_0 = 0$, at which $\phi(\theta)$ is always unity. Then, for $\theta = \theta_1$ (> 0) close to $\theta = \theta_0$, check if

$$|\phi(\theta_0) + \tilde{\phi}(\theta_1)| \le |\phi(\theta_0) - \tilde{\phi}(\theta_1)|, \tag{6.4}$$

where $\tilde{\phi}(\theta_1)$ is the computer-generated value of $\phi(\theta_1)$. If (6.4) is true, it means that the computer has generated $\phi(\theta_1)$ with the wrong sign so that we put $\phi(\theta_1) = -\tilde{\phi}(\theta_1)$; otherwise we put $\phi(\theta_1) = \tilde{\phi}(\theta_1)$. Then we proceed to check if

$$|\phi(\theta_1) + \tilde{\phi}(\theta_2)| \le |\phi(\theta_1) - \tilde{\phi}(\theta_2)|, \tag{6.5}$$

for θ_2 ($> \theta_1$) close to θ_1. If (6.5) holds true, we put $\phi(\theta_2) = -\tilde{\phi}(\theta_2)$; otherwise we put $\phi(\theta_2) = \tilde{\phi}(\theta_2)$. Proceeding further in this way we can compute the correct c.f. $\phi(\theta)$ for successive values of θ. Figure 6.2 shows the graph of $\phi_1(\theta)$ in (6.3) computed in the way described above.

Figure 6.2

We now proceed to the computation of $F(x)$ in (6.1). For this purpose we need to examine the behavior of the integrand. Here we consider, by change of variables,

$$\begin{aligned} F_1(x) &= \frac{1}{\pi}\int_0^\infty \mathrm{Re}\left[\frac{1-e^{-i\theta x}}{i\theta}\,\phi_1(\theta)\right]d\theta \\ &= \frac{1}{\pi}\int_0^\infty g_1(u;\,x)du\,, \end{aligned} \tag{6.6}$$

where we have put $\theta = u^2$ and

$$g_1(u;\,x) = \mathrm{Re}\left[\frac{2(1-e^{-iu^2x})}{iu}\,\phi_1(u^2)\right]. \tag{6.7}$$

We have transformed θ into $\theta = u^2$ because $\phi_1(\theta)$ in (6.3) involves $\sqrt{\theta}$. If the c.f. involves $\theta^{1/m}$ ($m > 1$), we shall consider $\theta = u^m$. The transformed integrand $g_1(u;\,x)$ in (6.7) reduces to 0 at $u = 0$. Thus we can dispense with computing the value of the integrand at the origin. This is especially advantageous to the numerical integration dealt with in Section 3, where such computation is complicated.

Figure 6.3 shows the graph of the transformed integrand $g_1(u;\, x)$ in (6.6) for $0 \le u \le 10$ and $x = 0.74346$. The present value of x is supposed to be the upper 1% point. The computation of percent points will be explained in Section 5. We need to determine an effective interval where the integrand is nonnegligible. It turns out that the interval $0 \le u < \infty$ of the integral in (6.6) may be replaced by $0 \le u \le 50$ for the present and other moderate values of x. Simpson's rule will do a proper job for numerical integration in (6.6), which will be discussed later by presenting a Fortran program.

Figure 6.3

The computation of the probability density $f(x)$ in (6.2) proceeds in much the same way as above, once the correct c.f. is obtained. We transform the integrand to get

$$
(6.8) \qquad f_1(x) = \frac{1}{\pi}\int_0^\infty \mathrm{Re}\left[e^{-i\theta x}\phi_1(\theta)\right] d\theta = \frac{1}{\pi}\int_0^\infty h_1(u;\, x)du\,,
$$

where $\theta = u^2$ and

$$
(6.9) \qquad h_1(u;\, x) = \mathrm{Re}\left[2ue^{-iu^2 x}\phi_1(u^2)\right] .
$$

The transformed integrand $h_1(u;\, x)$ also vanishes at $u = 0$. The effective interval for which this integrand is nonnegligible is usually wider than that for the distribution function. Figure 6.4 shows the graph of $h_1(u;\, x)$ for $0 \le u \le 20$ and the same value of x as above. It is seen that, unlike the integrand in Figure 6.3, the present one is oscillating around zero and does not approach zero so rapidly. Simpson's rule, however, is found to be still applicable to the present situation, although we need a slightly wider effective interval for integration.

Figure 6.4

We are now ready to compute $F_1(x)$ in (6.6) and $f_1(x)$ in (6.8). *Simpson's rule* tells us that

$$
(6.10) \qquad I = \int_a^b f(u)du
$$

$$= \frac{h}{3}\left[4\sum_{i=1}^{n} f(u_{2i-1}) + 2\sum_{i=1}^{n-1} f(u_{2i}) + f(a) + f(b)\right],$$

where $h = (b-a)/(2n)$ and $u_i = a + ih$. In the present case $a = 0$ and $f(u) = g_1(u;\, x)$ or $h_1(u;\, x)$. Note that $g_1(0;\, x) = h_1(0;\, x) = 0$ so that these terms do not contribute to the above sum.

Table 6.1 presents a Fortran program for computing $F_1(x)$ and $f_1(x)$ for $x = 0.01\,(+0.01)\,1.2$. In this program we have chosen $b = M = 50$, $1/h = N = 50$ and $2n = L = 2,500$. It is desirable to try various values of $h = 1/N$ to ensure that the result do not depend on those values. The values of $f_1(x)$ may be used to draw the graph of the probability density, but some more finer points of x will be necessary to get a correct graph. Such a graph was already presented in Chapter 1 as part of Figure 1.2.

Table 6.1

In Chapter 5 we have presented various c.f.'s for nonnegative statistics. The distribution functions and the probability densities of most of those statistics may be computed by the present method. The only exception is the statistic involving the integrated Brownian motion. A simple application of Simpson's rule does not accomplish the job properly since it is found that the associated integrand is oscillating and converges to 0 rather slowly. This will be discussed in the next section.

For c.f.'s that contain Bessel functions together with gamma functions presented in Section 4 of Chapter 5 we can usually make use of a computer package for computing those functions. MacNeill (1974, 1978) and Nabeya and Tanaka (1988) dealt with such cases. Simpson's rule is found to be applicable in those cases.

6.3. Numerical integration : the oscillating case

Here we take up examples for which a simple application of Simpson's rule fails. We suggest using Euler's transformation to overcome the difficulty. Another practical remedy will be given in the next section.

As the first example let us consider

$$(6.11) \qquad S_2 = \int_0^1\int_0^1 [\, dw_1(s)dw_1(t) - dw_2(s)dw_2(t)\,]$$

$$= \int_0^1 \int_0^1 dw'(s) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} dw(t)\,,$$

where $w(t) = (w_1(t),\, w_2(t))'$ is the two-dimensional standard Brownian motion. Of course, $\mathcal{L}(S_2) = \mathcal{L}(X^2 - Y^2)$, where $(X,Y)' \sim \mathrm{N}(0, I_2)$. This observation leads us to take a more efficient method for computing the distribution function and the probability density of S_2, which will be considered later. We first stick to the method discussed so far.

The c.f. of S_2 is given by

$$\phi_2(\theta) = (1 + 4\theta^2)^{-\frac{1}{2}}\,. \tag{6.12}$$

The distribution of S_2 is certainly symmetric around the origin since the c.f. is real. Thus we need not worry about computing the square root of a complex-valued function. Imhof's (1961) formula gives us

$$\begin{aligned} F_2(x) &= P(S_2 \le x) \\ &= \frac{1}{2} - \frac{1}{\pi}\int_0^\infty \frac{1}{\theta}\,\mathrm{Im}\left[e^{-i\theta x}\phi_2(\theta)\right] d\theta \\ &= \frac{1}{2} + \frac{1}{\pi}\int_0^\infty \frac{\sin\theta x}{\theta\sqrt{1+4\theta^2}}\, d\theta\,, \end{aligned} \tag{6.13}$$

$$\begin{aligned} f_2(x) &= \frac{dF_2(x)}{dx} \\ &= \frac{1}{\pi}\int_0^\infty \frac{\cos\theta x}{\sqrt{1+4\theta^2}}\, d\theta\,. \end{aligned} \tag{6.14}$$

The integrands above take a simple form and one might think that Simpson's rule would execute numerical integration properly. This is not the case, however. This is because the integrands are oscillating and converges to 0 quite slowly. In particular the integrand involved in (6.14) is of order $1/\theta$ as $\theta \to \infty$. Change of variables like $\theta = u^2$ does not improve this situation.

Figure 6.5 shows a graph of

$$g_2(\theta;\, x) = \frac{\cos\theta x}{\sqrt{1+4\theta^2}}\,, \tag{6.15}$$

for $x = 3$. The function is oscillating around 0 and leaves rippling waves as far as $\theta = 100$ and beyond that point.

Figure 6.5

In the present case, however, we have another expression for $F_2(x)$ and $f_2(x)$. It can be shown (Problem 3.1) that, for $x \geq 0$,

$$(6.16) \qquad \begin{aligned} F_2(x) &= P(S_2 \leq x) = P(X^2 - Y^2 \leq x) \\ &= 1 - \frac{4}{\sqrt{2\pi}} \int_0^\infty \Phi(-\sqrt{x+\theta^2}) e^{-\theta^2/2} d\theta \,, \end{aligned}$$

and $F_2(x) = 1 - F_2(-x)$ for $x < 0$, where $(X, Y)' \sim \mathrm{N}(0, I_2)$ and $\Phi(\cdot)$ is the distribution function of $\mathrm{N}(0,1)$. Thus, for $x \geq 0$,

$$(6.17) \qquad f_2(x) = \frac{1}{\pi} \int_0^\infty \frac{1}{\sqrt{x+\theta^2}} \exp\left(-\frac{x}{2} - \theta^2\right) d\theta \,,$$

and $f_2(x) = f_2(-x)$ for $x < 0$.

Figure 6.6 shows the graph of

$$(6.18) \qquad h_2(\theta;\, x) = \frac{1}{\sqrt{x+\theta^2}} \exp\left(-\frac{x}{2} - \theta^2\right)$$

for $x = 3$. It is to be recognized that the integration based on (6.17) gives a more efficient method for computing $f_2(x)$ than that based on (6.14). Simpson's rule or any other computer package can be used for numerical integration in (6.16) and (6.17). Note, however, that $f_2(x)$ diverges as $|x| \to 0$ so that, in drawing the graph of $f_2(x)$, the integration in (6.17) should be done for various values of x excluding $x = 0$. The probability density of $S_2/2$, that is, $f(x) = 2f_2(2x)$ was already presented in Figure 1.4.

Figure 6.6

In general it is not easy to find an alternative expression for integration which is computationally more efficient. As such an example we consider the integral of the square of the one-fold integrated Brownian motion :

$$(6.19) \qquad S_3 = \int_0^1 \left\{ \int_0^t w(s) ds \right\}^2 dt \,,$$

whose c.f. is available from (4.42) or (5.89) as

$$(6.20) \qquad \phi_3(\theta) = \left[\frac{1}{2} \left\{ 1 + \cos(2i\theta)^{\frac{1}{4}} \cosh(2i\theta)^{\frac{1}{4}} \right\} \right]^{-\frac{1}{2}} .$$

Figure 6.7 draws $\phi_3(u^4)$ as a function of u.

Figure 6.7

Lévy's inversion formula (6.1) leads us (Problem 3.2) to

$$
\begin{aligned}
(6.21)\qquad F_3(x) &= P(S_3 \le x) \\
&= \frac{1}{\pi}\int_0^\infty g_3(u;\, x)du\,,
\end{aligned}
$$

where we have put $\theta = u^4$ in (6.20) and

$$
(6.22)\qquad g_3(u;\, x) = \frac{4}{u}\left[\mathrm{Re}\left\{\phi_3(u^4)\right\}\sin u^4x + \mathrm{Im}\left\{\phi_3(u^4)\right\}(1-\cos u^4x)\right]\,.
$$

We also have the probability density given by

$$
(6.23)\qquad f_3(x) = \frac{1}{\pi}\int_0^\infty h_3(u;\, x)du\,,
$$

where

$$
(6.24)\qquad h_3(u;\, x) = 4u^3\left[\mathrm{Re}\left\{\phi_3(u^4)\right\}\cos u^4x + \mathrm{Im}\left\{\phi_3(u^4)\right\}\sin u^4x\right]\,.
$$

Figures 6.8 and 6.9 present graphs of $g_3(u;\, x)$ and $h_3(u;\, x)$, respectively, for $x = 0.3$. It turns out that Simpson's rule fails even in the computation of the former, much more the latter.

Figure 6.8 Figure 6.9

To overcome the difficulty we use *Euler's transformation* of slowly convergent alternating series (Longman (1956)). Suppose that the integrand $f(u)$ defined on $[0, \infty)$ has zeros at $u = u_k$ $(k = 1, 2, \cdots)$. Then we have

$$
\begin{aligned}
(6.25)\qquad I &= \int_0^\infty f(u)du \\
&= \int_0^{u_1} f(u)du + \int_{u_1}^{u_2} f(u)du + \cdots \\
&= \sum_{k=0}^{\infty}(-1)^k V_k\,,
\end{aligned}
$$

where

$$
V_k = (-1)^k\int_{u_k}^{u_{k+1}} f(u)du\,, \qquad (u_0 = 0)\,.
$$

By definition $\{(-1)^k V_k\}$ is an alternating series. It can be shown (Problem 3.3) that

$$
\begin{aligned}
(6.26) \qquad I &= \sum_{k=0}^{\infty}(-1)^k V_k \\
&= \sum_{k=0}^{\infty}(-1)^k \frac{(F-1)^k V_0}{2^{k+1}} \\
&= \sum_{k=0}^{N-1}(-1)^k V_k + \sum_{k=0}^{\infty}(-1)^{k+N} \frac{(F-1)^k V_N}{2^{k+1}} \,,
\end{aligned}
$$

where F is the forward shift operator, that is, $FV_k = V_{k+1}$ and

$$
(6.27) \qquad (F-1)^k V_j = (F-1)^{k-1}(V_{j+1} - V_j)\,, \quad (F-1)^0 V_j = V_j\,.
$$

Euler's transformation refers to the second relation in (6.26). The third may be referred to as Euler's delayed transformation. Since each V_k has the same sign and $\{|V_k|\}$ is supposed to be a decreasing sequence, it is expected that the k-fold forward difference $(F-1)^k V_N$ of V_N divided by 2^{k+1} makes the convergence of the infinite series more rapid. Each V_k is easily computed by Simpson's rule.

Returning to the integral in (6.21) we need to find the zeros of the integrand $g_3(u;\, x)$. It is, however, not easy. Thus we split $g_3(u;\, x)$ into $g_3(u;\, x) = a(u;\, x) - b(u;\, x) + c(u)$ where

$$
\begin{aligned}
(6.28) \qquad a(u;\, x) &= \frac{4}{u}\,\mathrm{Re}[\phi_3(u^4)]\sin u^4 x\,, \\
(6.29) \qquad b(u;\, x) &= \frac{4}{u}\,\mathrm{Im}[\phi_3(u^4)]\cos u^4 x\,, \\
(6.30) \qquad c(u) &= \frac{4}{u}\,\mathrm{Im}[\phi_3(u^4)]\,.
\end{aligned}
$$

Figures 6.10, 6.11 and 6.12 present graphs of $a(u;\, x)$ and $b(u;\, x)$ for $x = 0.3$, and $c(u)$, respectively. It is expected that the integral of $c(u)$ is easily done by Simpson's rule. As for the integrals of $a(u;\, x)$ and $b(u;\, x)$ we apply Euler's transformation (6.26) to the sequence of values of integrals computed by Simpson's rule, noting that the zeros of $a(u;\, x)$ are $u_k = (k\pi/x)^{\frac{1}{4}}$, while those of $b(u;\, x)$ are $\left\{\left(k+\frac{1}{2}\right)\pi/x\right\}^{\frac{1}{4}}$ for $k = 0, 1, \cdots$, apart from the zeros of $\phi_3(u^4)$.

Figure 6.10 Figure 6.11 Figure 6.12

Once the c.f. $\phi_3(\theta)$ is computed, the computation of the integrals of $a(u;\, x)$ and $b(u;\, x)$ in the way described above is easily programed, which will be presented in Section 5 in connection with computing percent points.

Because of the nature of the function $h_3(u;\, x)$ presented in Figure 6.9, the computation of $f_3(x)$ in (6.23) by the above method is found to be not very accurate. Since we can compute $F_3(x)$ quite accurately, it is expected that $f_3(x)$ can be obtained, to a certain degree of accuracy, from numerical derivatives of $F_3(x)$. This will be a topic in the next section, where the graph of $f_3(x)$ computed in that way is presented.

Here we just content ourselves with observing that the present method is also applicable to compute the distribution function of

$$S_4 = \int_0^1 \left[\int_0^t \left\{ \int_0^s w(r)dr \right\} ds \right]^2 dt\,, \tag{6.31}$$

where the integrand is the square of the two-fold integrated Brownian motion. It follows from (5.91) that the c.f. of S_4 is given by

$$\begin{aligned} \phi_4(\theta) \quad = \quad & \left[\frac{1}{18} \left\{ \left(\cos\mu + 2\cosh^2 \frac{\sqrt{3}\mu}{2} + 3 \right) \cos\mu \right.\right. \\ & \left.\left. \qquad + \, 8\cos\frac{\mu}{2} \cosh\frac{\sqrt{3}\mu}{2} + 4 \right\} \right]^{-\frac{1}{2}}, \end{aligned} \tag{6.32}$$

where $\mu = (2i\theta)^{\frac{1}{6}}$.

Figure 6.13 shows graphs of the distribution functions of S_3 in (6.19) and S_4 in (6.31). Percent points of these distributions will be tabulated in Section 5 together with a Fortran program.

Figure 6.13

Problems

3.1 Establish (6.16) when $(X, Y)' \sim \mathrm{N}(0, I_2)$.

3.2 Derive the second equality in (6.21).

3.3 Derive Euler's transformation as in (6.26).

6.4. Numerical integration : the general case

In this section we deal with statistics that take both positive and negative values. As a simple example in terms of numerical integration, let us first consider Lévy's stochastic area defined by

$$S_5 = \frac{1}{2}\int_0^1 [\, w_1(t)dw_2(t) - w_2(t)dw_1(t)\,]\,, \tag{6.33}$$

where $w(t) = (w_1(t),\, w_2(t))'$ is the two-dimensional standard Brownian motion. The c.f. of S_5 is available from (1.57) or (5.38), which is

$$\phi_5(\theta) = E\left(e^{i\theta S_5}\right) = \left(\cosh\frac{\theta}{2}\right)^{-1}\,. \tag{6.34}$$

The statistic S_5 has a symmetric distribution since $\phi_5(\theta)$ is real. Thus we need not worry about computing the square root of a complex-valued function. In fact Imhof's formula described in (6.13) gives us

$$\begin{aligned} F_5(x) &= P(S_5 \le x) \\ &= \frac{1}{2} + \frac{1}{\pi}\int_0^\infty \frac{\sin\theta x}{\theta\cosh\frac{\theta}{2}}\,d\theta\,. \end{aligned} \tag{6.35}$$

The integrand $\sin\theta x/\left(\theta\cosh\dfrac{\theta}{2}\right)$ takes the value x at $\theta = 0$. Any computer package will compute the above integral fairly easily. The computation of the probability density given by

$$f(x) = \frac{1}{\pi}\int_0^\infty \frac{\cos\theta x}{\cosh\frac{\theta}{2}}\,d\theta$$

is also easy since the integrand approaches 0 exponentially. The graph of the probability density of $2 \times S_5$ was earlier presented in Figure 1.4 with percent points in Table 1.4.

We now deal with statistics for which numerical integration must be elaborated. Let S be such a statistic, which takes the form $S = U/V$, where $P(V > 0) = 1$. Imhof's formula for such a statistic gives us

$$\begin{aligned} F(x) &= P(S \le x) \\ &= P(xV - U \ge 0) \\ &= \frac{1}{2} + \frac{1}{\pi}\int_0^\infty \frac{1}{\theta}\,\mathrm{Im}\,[\,\phi(\theta;\, x)]\,d\theta\,, \end{aligned} \tag{6.36}$$

where $\phi(\theta;\, x)$ is the c.f. of $xV - U$. In actual computation we shall transform θ into another variable to make the integrand vanish at the origin, as was done in previous sections.

If $F(x)$ is differentiable, we have

$$(6.37)\qquad f(x) = \frac{dF(x)}{dx} = \frac{1}{\pi}\int_0^\infty \frac{1}{\theta}\,\mathrm{Im}\left[\frac{\partial\phi(\theta;\, x)}{\partial x}\right] d\theta\,.$$

Here it is usually the case that $\phi(\theta;\, x)$ is a complicated function of x, which makes the computation of $\partial\phi(\theta;\, x)/\partial x$ tedious. It is also the case, as was seen in the last section, that the integration for computing probability densities is more difficult than for distribution functions. Even if we use Euler's transformation, we require the values of θ for which $\partial\phi(\theta;\, x)/\partial x = 0$. It is also difficult in the present case. We, however, only need the values of $f(x)$ to draw its graph; hence very accurate values of $f(x)$ are not our concern.

The above discussions lead us to dispense with the computation of $f(x)$ that follows (6.37). Instead we proceed as follows. Let $F(x)$ and $F(x + \Delta x)$ be already computed by following (6.36), where Δx is a small number, 10^{-6}, say. Then we suggest computing $f(x)$ as

$$(6.38)\qquad f(x) = \frac{F(x + \Delta x) - F(x)}{\Delta x}\,.$$

The right side above is a numerical derivative of $F(x)$. Computing $f(x)$ in this way we can also avoid examining the behavior of the integrand associated with numerical integration in (6.37). We have only to concentrate on the computation of $F(x)$ discussed in the previous sections.

As an example let us consider the statistic S_6 given by

$$(6.39)\qquad S_6 = \frac{U_6}{V_6} = \frac{\displaystyle\int_0^1 w(t)dw(t)}{\displaystyle\int_0^1 w^2(t)dt}\,,$$

which follows the AR(1) unit root distribution discussed in Section 3 of Chapter 1. An extended version of S_6 was discussed in Section 1 of Chapter 4. We have

$P(S_6 \le x) = P(xV_6 - U_6 \ge 0)$, and (1.35) or (4.17) yields

$$\text{(6.40)} \qquad \begin{aligned} \phi_6(\theta;\, x) &= E\left[\exp\{i\theta(xV_6 - U_6)\}\right] \\ &= e^{i\theta/2}\left[\cos\sqrt{2i\theta x} + i\theta\,\frac{\sin\sqrt{2i\theta x}}{\sqrt{2i\theta x}}\right]^{-\frac{1}{2}} . \end{aligned}$$

The c.f. $\phi_6(\theta;\, x)$ can be obtained (Problem 4.1) most easily by the stochastic process approach discussed in Chapter 4.

Putting $\theta = u^2$ we consider

$$\text{(6.41)} \qquad \begin{aligned} F_6(x) &= P(S_6 \le x) \\ &= \frac{1}{2} + \frac{1}{\pi}\int_0^\infty g_6(u;\, x)du\,, \end{aligned}$$

where

$$\text{(6.42)} \qquad g_6(u;\, x) = \frac{2}{u}\,\mathrm{Im}\left[\phi_6(u^2;\, x)\right] .$$

Note that $g_6(0;\, x) = 0$ (Problem 4.2) so that we can dispense with computing the value of the integrand at the origin. If we follow the untransformed formula (6.36), we need (Problem 4.3)

$$\text{(6.43)} \qquad \lim_{\theta\to 0}\frac{1}{\theta}\,\mathrm{Im}\left[\phi_6(\theta;\, x)\right] = \frac{x}{2}\,.$$

Figure 6.14 gives the graph of the integrand $g_6(u;\, x)$ in (6.41) for $x = -8.03913$. The present value of x is supposed to be the 5% point of the distribution of S_6 in (6.39). It is expected that the numerical integration for (6.41) with the present value of x can be easily done by Simpson's rule. On the other hand, Figure 6.15 shows the graph of $g_6(u;\, x)$ for $x = 0.05$. This graph is quite different from that in Figure 6.14; the integrand is oscillating and converges slowly to 0. This is because $|x|$ is quite small. In fact, if $x = 0$, the integrand (6.42) becomes

$$g_6(u;\, 0) = \frac{2}{u}\,\mathrm{Im}\left[\frac{e^{iu^2/2}}{\sqrt{1+iu^2}}\right] ,$$

which is of a similar nature to the integrand in (6.13). Of course we can take another route to evaluate $F_6(0)$ more efficiently (Problem 4.4). For cases of $|x|$ ($\ne 0$) small we can still use Simpson's rule since the rate of convergence of the integrand to 0 is not very slow, although the effective interval of the integral in (6.41) becomes wider.

Figure 6.14 Figure 6.15

Table 6.2 presents a Fortran program for computing $F_6(x)$ and $f_6(x)$ for $x = -14.5\,(+1)\,2.5$, where the computation of $f_6(x)$ is done by numerical derivatives of $F_6(x)$ as in (6.38) with $\Delta x = \text{DINC} = 10^{-6}$. As for the parameters used in Simpson's rule (6.10), we have chosen $b = M = 30$, $1/h = N = 100$ and $2n = L = 3,000$. The graph of $f_6(x)$ was already presented in Chapter 1 as part of Figure 1.3.

Table 6.2

As another example we take up

$$(6.44) \qquad S_7 = \frac{U_7}{V_7} = \frac{\displaystyle\int_0^1 \left\{ \int_0^t w_1(s)ds \right\} dw_2(t)}{\displaystyle\int_0^1 \left\{ \int_0^t w_1(s)ds \right\}^2 dt},$$

where $w(t) = (w_1(t),\, w_2(t))'$ is the two-dimensional standard Brownian motion. The statistic S_7 was earlier given in (4.48) and may be interpreted as the limit in distribution of the LSE arising from the second-order cointegrated process described in (4.51). It follows from (4.49) that the c.f. of $xV_7 - U_7$ is given by

$$(6.45) \qquad \phi_7(\theta;\, x) = \left[\frac{1}{2} \left\{ 1 + \cos(2i\theta x - \theta^2)^{\frac{1}{4}} \cosh(2i\theta x - \theta^2)^{\frac{1}{4}} \right\} \right]^{-\frac{1}{2}}.$$

Putting here $\theta = u^4$ we obtain

$$(6.46) \qquad \begin{aligned} F_7(x) &= P(S_7 \le x) \\ &= \frac{1}{2} + \frac{1}{\pi} \int_0^\infty g_7(u;\, x)du\,, \end{aligned}$$

where

$$(6.47) \qquad g_7(u;\, x) = \frac{4}{u} \,\text{Im}\left[\phi_7(u^4;\, x) \right]$$

with $g_7(0;\, x) = 0$.

Figure 6.16 gives the graph of $g_7(u;\, x)$ for $x = -14.8468$. The present value of x is supposed to be the 5% point of the distribution of S_7 in (6.44). Although not presented here, the integrand $g_7(u;\, x)$ performs well even for $|x|$ small. In fact, if

$x = 0$, $g_7(u;\, x)$ reduces to zero (Problem 4.5) so that $F_7(0) = \dfrac{1}{2}$. It can also be shown (Problem 4.6) that the distribution of S_7 is symmetric about the origin. The integration for (6.46) can be easily done by Simpson's rule for all moderate values of x.

Figure 6.16

As far as the computation of probability densities is based on numerical derivatives of distribution functions, we do not have to worry about the integration associated with probability densities. We have only to compute $F(x + \Delta x)$ as well as $F(x)$ for each x to obtain $f(x)$ as in (6.38). In subsequent chapters we shall always use numerical derivatives whenever graphs of probability densities are presented. Here, as a sequel to the last section, the graphs of probability densities of S_3 in (6.19) and S_4 in (6.31) are presented in Figures 6.17 and 6.18, respectively. Also shown in each figure is an approximation by a constant multiple of $\chi^2(1)$ distribution discussed in Section 4 of Chapter 5, that is

$$\begin{aligned} \mathcal{L}(S_3) &\sim \mathcal{L}\left(\frac{1}{12.36236}\, Z^2\right), \\ \mathcal{L}(S_4) &\sim \mathcal{L}\left(\frac{1}{121.259}\, Z^2\right), \end{aligned}$$

where $Z \sim \mathrm{N}(0, 1)$.

Figure 6.17 Figure 6.18

Problems

4.1 Derive the c.f. of $xV_6 - U_6$ by the stochastic process approach, where U_6 and V_6 are defined in (6.39).

4.2 Show that $g_6(u;\, x)$ in (6.42) is equal to 0 when $u = 0$.

4.3 Establish the relation in (6.43).

4.4 Derive the easiest way of computing $F_6(x)$ in (6.41) when $x = 0$ and obtain its value.

4.5 Prove that $g_7(u; x)$ in (6.47) reduces to 0 if $x = 0$.

4.6 Show that the distribution of S_7 in (6.44) is symmetric about the origin.

6.5. Computation of percent points

For testing purposes it is necessary to obtain percent points. Since we have learned, to a large extent, how to compute distribution functions, the task of computing percent points is almost its byproduct. Here we present two methods for computing percent points on the basis of distribution functions.

Suppose that we would like to find the $100\alpha\%$ point of $F(x)$, that is, the value x such that $F(x) = \alpha$. For this purpose we first consider *Newton's method of successive approximation* :

$$x_i = x_{i-1} - \frac{F(x_{i-1}) - \alpha}{f(x_{i-1})}, \qquad (i = 1, 2, \cdots), \tag{6.48}$$

where x_0 is a starting value such that $F(x_0)$ is close to α, while $f(x) = dF(x)/dx$ or $f(x) = (F(x + \Delta x) - F(x))/\Delta x$ with Δx small, $\Delta x = 10^{-6}$, say. The above iteration may be terminated when $|x_i - x_{i-1}|$ becomes small for $i = n$, at which the $100\alpha\%$ point of $F(x)$ is obtained as x_n.

Another method for computing percent points is the *bisection method.* Let x_1 and x_2 be close to the solution to $F(x) = \alpha$, where $F(x_1) < \alpha$ and $F(x_2) > \alpha$. Then we compute $F(x)$ for $x = \bar{x} = (x_1 + x_2)/2$. If $F(\bar{x}) < \alpha$, then we replace x_1 by $\bar{x}$; otherwise we replace x_2 by $\bar{x}$. We again compute $F(x)$ for the mean of the newly defined values x_1 and x_2. This procedure is iterated until $|x_2 - x_1|$ becomes smaller than a preassigned level. In comparison with Newton's method the present one needs less computation and avoids the computation of derivatives of $F(x)$, although the number of iterations required to attain convergence may be larger.

As an examle we take up again the distribution of S_3 in (6.19). A Fortran program which computes various percent points are presented in Table 6.3, where the bisection method is used together with Euler's transformation along the lines discussed in Section 3. Table 6.4 tabulates percent points of S_3 computed in this way together with those of S_4 in (6.31).

Table 6.3   Table 6.4

Various tables presented in Chapter 1 were also tabulated by either Newton's method or the bisection method. We shall further present percent points of other distributions in later chapters.

6.6. The saddlepoint approximation

If our purpose is just to obtain approximations to distribution functions or percentiles, the *saddlepoint method* enables us to compute those without employing any numerical integration method. Daniels (1954) first introduced this method into statistics. For our purpose we find the approach taken by Helstrom (1978) useful, which we now describe.

Let $\phi(\theta)$ be the c.f. of a random variable S, and $F(x)$ its distribution function. To make the presentation simpler we assume here that S takes only nonnegative values and is a quadratic functional of the Brownian motion. We then put

$$(6.49) \qquad h(z) = \phi(-iz) = E\left(e^{zS}\right),$$

where z is a complex variable. When z is real, $h(z)$ is the m.g.f. of S.

Helstrom (1978) recommends to determine $F(x)$ following

$$(6.50) \qquad F(x) = \frac{1}{2\pi i}\int_{\bar{\theta}-i\infty}^{\bar{\theta}+i\infty}\left(-\frac{1}{z}\right)h(z)e^{-xz}dz\,, \quad \left(\theta_L < \bar{\theta} < 0\right)$$

for the left-hand tail and

$$(6.51) \qquad 1 - F(x) = \frac{1}{2\pi i}\int_{\bar{\theta}-i\infty}^{\bar{\theta}+i\infty}\frac{1}{z}h(z)e^{-xz}dz\,, \quad \left(0 < \bar{\theta} < \theta_R\right)$$

for the right-hand tail, where θ_L is the first singularity point of $h(\theta)$ to the left of the origin, while θ_R is that of $h(\theta)$ to the right of the origin. Note that the singularity points of $h(\theta)$ are all positive because of the assumption on S. Thus we may put $\theta_L = -\infty$ in the present case. If S is a nonpositive random variable, the role of θ_L and θ_R should be interchanged. If S takes both positive and negative values, the choice of $\bar{\theta}$ cannot be made in advance. This is a main reason why we assume S to be a nonnegative random variable. We cannot usually rely only on (6.50) or (6.51) to obtain good approximations, as is shown later by an illustrative example. For a given value of x, however, it is somewhat arbitrary whether we should use (6.50) or (6.51). A graphical solution will be given later. As the value of $\bar{\theta}$ we shall take the saddlepoint of the integrand in each of (6.50) and (6.51), which we now discuss.

Let us consider the logarithm of the integrand in (6.50) on the negative real axis :

$$\text{(6.52)} \qquad \Psi_-(\theta; x) = \log h(\theta) - \theta x - \log(-\theta)\,, \qquad (\theta < 0)\,.$$

Since $\exp\{\Psi_-(\theta; x)\}$ is shown to be convex for any x, $\Psi_-(\theta; x)$ is expected to have a single minimum. If this is the case, the minimizer is a solution to

$$\text{(6.53)} \qquad \Psi_-^{(1)}(\theta; x) \equiv \frac{\partial \Psi_-(\theta; x)}{\partial \theta} = \frac{1}{h(\theta)}\frac{dh(\theta)}{d\theta} - x - \frac{1}{\theta} = 0\,, \qquad (\theta < 0)\,.$$

The solution is called the *saddlepoint* of the complex-valued function $h(z)e^{-xz}/(-z)$, and is denoted by θ_-. The assumption that $\theta_L < \theta_- < 0$ is ensured in the present case.

Similarly, if we consider

$$\text{(6.54)} \qquad \Psi_+(\theta; x) = \log h(\theta) - \theta x - \log \theta\,, \qquad (\theta > 0)\,,$$

the saddlepoint of the integrand $h(z)e^{-xz}/z$ in (6.51) is a solution to

$$\text{(6.55)} \qquad \Psi_+^{(1)}(\theta; x) \equiv \frac{\partial \Psi_+(\theta; x)}{\partial \theta} = \frac{1}{h(\theta)}\frac{dh(\theta)}{d\theta} - x - \frac{1}{\theta} = 0\,, \qquad (\theta > 0)\,.$$

This solution is denoted by θ_+, for which we assume $0 < \theta_+ < \theta_R$.

Expanding $\exp\{\Psi_-(z; x)\}$ with $z = \theta_- + i\theta$ around θ_- we have

$$\begin{aligned} \exp\{\Psi_-(z; x)\} &= h(z)e^{-xz}/(-z) \\ &\cong \exp\left\{\Psi_-(\theta_-; x) - \frac{1}{2}\Psi_-^{(2)}(\theta_-)\theta^2\right\}\,, \end{aligned}$$

where

$$\Psi_*^{(2)}(\theta_*) = \left.\frac{\partial^2 \Psi_*(\theta; x)}{\partial \theta^2}\right|_{\theta = \theta_*}\,.$$

Substituting this into (6.50) with $\bar{\theta} = \theta_-$ we obtain the saddlepoint approximation to $F(x)$:

$$F(x) \cong \frac{1}{2\pi} \exp\{\Psi_-(\theta_-; x)\} \int_{-\infty}^{\infty} \exp\left\{-\frac{1}{2}\Psi_-^{(2)}(\theta_-)\theta^2\right\} d\theta = \frac{1}{\sqrt{2\pi\Psi_-^{(2)}(\theta_-)}} \exp\{\Psi_-(\theta_-; x)\}\,. \tag{6.56}$$

Similarly, we obtain

$$1 - F(x) \cong \frac{1}{\sqrt{2\pi\Psi_+^{(2)}(\theta_+)}} \exp\{\Psi_+(\theta_+; x)\}\,. \tag{6.57}$$

Once x is given, θ_- and θ_+ can be found by Newton's method. Then we can compute the saddlepoint approximate distribution following (6.56) or (6.57).

As an example let us take up the c.f. $\phi(\theta) = \left(\sin\sqrt{2i\theta}/\sqrt{2i\theta}\right)^{-\frac{1}{2}}$ so that

$$\begin{aligned} h(\theta) &= \left(\frac{\sinh\sqrt{-2\theta}}{\sqrt{-2\theta}}\right)^{-\frac{1}{2}}, \qquad (\theta < 0)\,, \\ &= \left(\frac{\sin\sqrt{2\theta}}{\sqrt{2\theta}}\right)^{-\frac{1}{2}}, \qquad (\theta > 0)\,. \end{aligned} \tag{6.58}$$

It follows that $\theta_L = -\infty$ and $\theta_R = \pi^2/2 = 4.9348$.

Table 6.5 reports saddlepoints θ_- and θ_+ associated with (6.58) for some selected values of x. Also shown are approximate probabilities P_- and P_+ computed from (6.56) and (6.57), respectively, together with the exact probability P based on Simpson's rule. It is seen that the saddlepoints are increasing as x becomes large, but they are all smaller than θ_R. It is also observed that P_- behaves quite well on the left-hand tail, while P_+ on the right-hand tail. Neither P_- nor P_+ approximates P well for the whole range of x.

Table 6.5

Figure 6.19 is a graphical version of Table 6.5. The two approximate distributions cross each other at $x = 0.26$. Thus we recommend in the present case that P_- be used for $x \leq 0.26$ and P_+ for $x > 0.26$.

Figure 6.19

The saddlepoint approximate percentiles can be obtained as follows. Suppose that $F(x) = \alpha$ is given. Then, noting that

$$x = \frac{1}{h(\theta)} \frac{dh(\theta)}{d\theta} - \frac{1}{\theta} \tag{6.59}$$

at $\theta = \theta_-$, and substituting this into (6.52), it follows from (6.56) that θ_- must be approximately a solution to

$$\log \alpha = \log h(\theta) - \frac{\theta}{h(\theta)} \frac{dh(\theta)}{d\theta} + 1 - \log(-\theta) - \frac{1}{2} \log \left\{ 2\pi \Psi_-^{(2)}(\theta) \right\} , \tag{6.60}$$

where $\theta < 0$. Similarly, if $1 - F(x) = 1 - \beta$ is given, θ_+ must be approximately a solution to

$$\log(1-\beta) = \log h(\theta) - \frac{\theta}{h(\theta)} \frac{dh(\theta)}{d\theta} + 1 - \log \theta - \frac{1}{2} \log \left\{ 2\pi \Psi_-^{(2)}(\theta) \right\} , \tag{6.61}$$

where $\theta > 0$. The equations (6.60) and (6.61) can be most efficiently solved for θ by the *secant method*. Then percent points are obtained from (6.59) with θ replaced by the solution to (6.60) or (6.61).

The saddlepoints need not be computed accurately since (6.60) and (6.61) are just an approximation. The following examples also indicate that percent points computed from (6.59) are insensitive to a small departure from the solution to (6.60) or (6.61).

Let us take up two examples : one has the m.g.f. defined in (6.58); and the other defined by

$$\begin{aligned} h(\theta) &= \left[\frac{1}{2} + \frac{1}{4} \left\{ \cos \sqrt{2}(-2\theta)^{\frac{1}{4}} + \cosh \sqrt{2}(-2\theta)^{\frac{1}{4}} \right\} \right]^{-\frac{1}{2}} , \qquad (\theta < 0) , \\ &= \left[\frac{1}{2} \left\{ 1 + \cos(2\theta)^{\frac{1}{4}} \cosh(2\theta)^{\frac{1}{4}} \right\} \right]^{-\frac{1}{2}} , \qquad (\theta > 0) . \end{aligned} \tag{6.62}$$

Note that a random variable with the m.g.f. (6.62) is given in (6.19). It follows that $\theta_L = -\infty$ and $\theta_R = 12.36236$.

Table 6.6 reports approximate percentiles associated with (6.58) and (6.62) for $\alpha = 0.05$ and $\beta = 0.95$ computed in the way described above, together with the exact percentiles based on numerical integration. The entries under the heading 'θ' are those values around the solution to (6.60) or (6.61), while those under 'odds' are differences of the left from the right side in (6.60) or (6.61). Those values of θ which have odds equal to 0 are approximate saddlepoints and the corresponding values of x are approximate percentiles. We observe that the approximate percentiles coincide with the exact ones up to the first two effective figures, as far as percentiles examined here are concerned. It is also seen that percentiles are insensitive to a small departure from approximate saddlepoints.

Table 6.6

The saddlepoint method can be implemented to compute exact distribution functions and percent points. Helstrom (1995) also suggests that method, which we do not pursue in this book.