NUMERICAL INTEGRATION RULES FOR MULTIVARIATE INVERSIONS

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Working from a known characteristic function, integration rules for the computation of the multivariate distribution function are derived. Procedures for the automatic selection of step sizes are one particular strength of the proposed method. Examples of the use of the procedure are given.

KEY WORDS: Characteristic functions, numerical integration, inversion theorems, Imhof procedure, correlation coefficients

1. INTRODUCTION

In this paper we develop rules for the numerical inversion of multivariate characteristic functions in order to compute the distribution function. As such they represent multivariate generalisations of the Imhof (1961) and Davies (1973, 1980) techiques.

An example of the use of the multivariate inversion algorithm is discussed at length, while three other cases of its use are referenced.

2. THE UNIVARIATE CASE

We will suppose ϕ is a known characteristic function corresponding to the distribution function F which in turn possesses a density f. For ease of exposition we will assume f and ϕ are Lebesgue integrable and that the random variable of interest possesses a mean. These last three assumptions can be dropped without affecting our integration rules by using principle values of Lebesgue integrals, but we find that these types of details detract from the logical structure of our approach and so prefer to maintain our stated assumptions. These will allow us to develop the theory using standard manipulative techniques.

Gurland (1948) showed that F and ϕ are related in the following way

$$F(x) = \frac{1}{2} - \frac{1}{2\pi} \int_0^\infty \left(\Delta_t \left[\frac{\phi(t)e^{-itx}}{it} \right] \right) dt,$$

where $\Delta_t \eta(t) = \eta(t) + \eta(-t)$.

Following Davies (1973) we will rewrite this to give an expression which can be used to numerically invert characteristic functions. However, our proof is somewhat different from that used by Davies. Throughout the remaining parts of this paper we will exploit the operator $\delta(g, j)$ which is defined so that $\delta(g, j) \Pr(X \leq x) = \Pr(X \leq x - (2\pi j/h_g)) - \Pr(X > x + (2\pi j/h_g))$. In what follows h_g should be thought of as the step size of the integration procedure.

THEOREM 1 (Davies (1973))   *For $h_1 > 0$,*

$$F(x) + \sum_{j=1}^{\infty} \cos[2\pi z j] \left[\delta(1, j) \Pr(X \leq x)\right]$$

$$= \frac{1}{2} - \frac{1}{2\pi} h_1 \operatorname{Im}\left[\frac{\phi(h_1 z) \exp[-ixh_1 z]}{h_1 z}\right]$$

$$- \frac{1}{2\pi} h_1 \sum_{v=1}^{\infty} \left(\Delta_z \operatorname{Im}\left[\frac{\phi(h_1(z+v)) \exp[-ixh_1(z+v)]}{h_1(z+v)}\right]\right),$$

where $\operatorname{Im}(\cdot)$ *denotes the imaginary part of a complex function.*

Proof   Given in the appendix.

The second term of the left-hand side of this expression can be viewed as an error caused by approximating the inversion integral.

Allowing z to be zero means the integration is performed by the trapezium rule. As the induced integration error is

$$\left|\sum_{j=1}^{\infty} \left[\delta(1, j) \Pr(X \leq x)\right]\right|,$$

which is rather difficult to manipulate, this rule has not been used for this type of inversion. Instead the simpler Riemann sum has been exploited. This occurs when we allow $z = \frac{1}{2}$.

COROLLARY 1 (Davies (1973))   *For $h_1 > 0$,*

$$F(x) + \sum_{j=1}^{\infty} (-1)^j \left[\delta(1, j) \Pr(X \leq x)\right]$$

$$= \frac{1}{2} - \frac{1}{\pi} h_1 \sum_{v=0}^{\infty} \operatorname{Im}\left[\frac{\phi(h_1(v+\frac{1}{2})) \exp[-ixh_1(v+\frac{1}{2})]}{h_1(v+\frac{1}{2})}\right].$$

The induced numerical integration error is much simpler here. The absolute value of the error is,

$$\left| \sum_{j=1}^{\infty} (-1)^j [\delta(1, j) \Pr(X \leq x)] \right| \leq \max\left[F\left(x - \frac{2\pi}{h_1}\right), \ 1 - F\left(x + \frac{2\pi}{h_1}\right) \right].$$

In turn we can deduce an automatic criterion for the selection of h_1 so that this error is small. If ϕ is analytic then the corresponding moment generating function will exist. We will write it as M, then for small $u > 0$ we have (see Davies (1973)) $1 - F(x) \leq M(u) \exp(-ux)$. Writing $\psi(u) = \log M(u)$ and selecting $x = \psi'(u) = d\psi(u)/du$ implies we have $1 - F(\psi'(u)) \leq \exp(-u \cdot \psi'(u) + \psi(u))$. Equally $F(\psi'(u)) \leq \exp[\psi(-u) + u\psi'(u)]$. Therefore, by appropriate choice of h_1, we can bound this induced error by any small positive real ε.

This formulation has successfully been applied to the problem of finding the exact distribution function of a quadratic form in normal variables by Davies (1980).

3. THE BIVARIATE CASE

In this section we transfer the development given in Section 2 over to the case of a bivariate distribution function. From Gurland (1948) or more easily Shephard (1991) we have

$$u(x_1, x_2) = 4F(x_1, x_2) - 2[F(x_1) + F(x_2)] + 1$$

$$= \frac{2^2}{(2\pi)^2} \int_0^{\infty} \int_0^{\infty} \left(\Delta_{t_1} \cdot \Delta_{t_2} \left[\frac{\phi(t)e^{-ix't}}{it_1 it_2} \right] \right) dt_1 \, dt_2.$$

To make the notation in the theorem reasonably compact we will use $\sum_{j=0}^{\infty}$ to denote the double sum over the variables j_1 and j_2 which vary between zero and infinity, but never equal zero simultaneously.

THEOREM 2   *For* $h_1, h_2 > 0$

$$2^{-2} u(x_1, x_2) + \sum_{j=0}^{\infty} \left(\left[\prod_{k=1}^{2} \cos[2\pi z_k j_k] \delta(k, j_k) \right] F(x_1, x_2) \right)$$

$$= \frac{-\frac{1}{2}}{(2\pi)^2} h_1 h_2 \left[\sum_{v_2 = -\infty}^{\infty} \left(\Delta_{z_2} \operatorname{Re}\left[\frac{\phi(h_1 z_1, a_2) e^{-ix'(h_1 z_1, a_2)'}}{h_1 z_1 a_2} \right] \right) \right.$$

$$\left. + \sum_{v_1 = 1}^{\infty} \sum_{v_2 = -\infty}^{\infty} \left(\Delta_{z_1} \cdot \Delta_{z_2} \operatorname{Re}\left[\frac{\phi(a) e^{-ix'a}}{a_1 a_2} \right] \right) \right],$$

where $a = [h_1(z_1 + v_1), \ h_2(z_2 + v_2)]' = (a_1, a_2)'$.

Proof Given in the appendix.

COROLLARY 2   *For* $h_1, h_2 > 0$

$$2^{-2}u(x_1, x_2) + \sum_{j=0}^{\infty} \left(\left[\prod_{k=1}^{2} (-1)^{j_k} \delta(k, j_k) \right] F(x_1, x_2) \right)$$

$$= \frac{-2}{(2\pi)^2} h_1 h_2 \left[\sum_{v_1=0}^{\infty} \sum_{v_2=-\infty}^{\infty} \text{Re} \left[\frac{\phi(b_1, b_2) e^{-ix'b}}{b_1 b_2} \right] \right], \qquad (1)$$

where $b = (h_1(v_1 + \frac{1}{2}), h_2(v_2 + \frac{1}{2}))' = (b_1, b_2)'$.

The induced integration error is at most

$$\max \left(\left[1 - F\left(x_1 + \frac{2\pi}{h_1}\right) \right] + \left[1 - F\left(x_2 + \frac{2\pi}{h_2}\right) \right], \ F\left(x_1 - \frac{2\pi}{h_1}\right) + F\left(x_2 - \frac{2\pi}{h_2}\right) \right).$$

Thus, we can use the bounds employed in Section 2 to provide a way of selecting the step sizes, h_1 and h_2.

Although this integration error looks daunting, it is in fact in a very convenient form. This is because to evaluate $F(x_1, x_2)$ we would usually have to numerically compute $F(x_1)$ and $F(x_2)$, which means h_1 and h_2 have already been chosen by the univariate routines. These selected values will ensure that the error in the bivariate numerical integral is small.

4. BIVARIATE IMHOF PROCEDURE

Let us suppose that we are interested in the joint distribution of the two quadratic forms in form variables $y_1 = u'Au$ and $y_2 = u'Bu$ where A and B are $T \times T$ matrices and, for sake of simplicity, $u \sim N(0, I)$. The joint characteristic function of y_1 and y_2 is given by

$$\phi(t_1, t_2) = E \exp[i . u'(t_1 A + t_2 B)u]$$

$$= \prod_{j=1}^{T} (1 - 2i\lambda_j(t_1, t_2))^{-1/2},$$

where $\lambda_j(t_1, t_2)$ denotes the jth eigenvalue of the $(t_1 A + t_2 B)$ matrix. We will be able to use the analytic structure of the characteristic function to rewrite the right-hand side of (1) in a productive way. Using the arguments of Imhof (1961) we have

$$\varepsilon(t) = \arg[\phi(t)e^{-ix't}] = \left[\left(\frac{1}{2_j} \sum_{j=1}^{T} \arctan[2\lambda_j(t_1, t_2)] \right) - x't \right]$$

and

$$\gamma(t) = |\phi(t)e^{-ix't}| = \prod_{j=1}^{T} [1 + 4\lambda_j^2(t_1, t_2)]^{-1/4}.$$

Thus we see that $\text{Re}[\phi(b_1, b_2)\exp(-ix'b)] = \gamma(b_1, b_2)\cdot\cos[\varepsilon(b_1, b_2)]$.

If A and B do not commute the use of these expressions to evaluate $\phi(t_1, t_2)$ can be very expensive as eigenvalue calculations will be required each time t_1 and t_2 vary. An alternative sometimes available is to use the eigenvalue-free technique suggested by Shively, Ansley and Kohn (1990). This exploits the Kalman filter running in complex arithmetic to efficiently compute $\phi(t_1, t_2)$. Another approach has been suggested by Krishnaiah (1977, 1980) and Khatri *et al.* (1977) who proposed the use of asymptotic expansions to approximate the joint distribution function.

5. THE MULTIVARIATE CASE

The multivariate inversion formula given in Gurland (1948) and Shephard (1991) shows that

$$u(x) = \frac{(-2)^p}{(2\pi)^p} \int_0^\infty \cdots \int_0^\infty \left(\Delta_{t_1}\cdot\Delta_{t_2}\cdots\Delta_{t_p}\left[\frac{\phi(t)e^{-x't}}{it_1\ldots it_p}\right]\right)dt,$$

where

$$u(x) = 2^p F(x_1, \ldots, x_p) - 2^{p-1}[F(x_2, \ldots, x_p) + \cdots + F(x_1, \ldots, x_{p-2}, x_{p-1})]$$

$$+ 2^{p-2}[F(x_3, x_4, \ldots, x_p) + \cdots + F(x_1, \ldots, x_{p-3}, x_{p-2})] + \cdots + (-1)^p.$$

Theorem 2 now generalises in a straightforward way to deal with p variables. The resulting expression is not very compact and so we have not presented it here. Instead we give the formula corresponding to z being a half as this is gives a useful integration rule. Again we use the expression $\sum_{j=0}^\infty$ to stand for the sum over the variables $j_1, \ldots, j_p$, where these indexes vary between zero and infinity, but never all equal zero simultaneously. Corollary 3 is the result.

COROLLARY 3 *For* $h_1, h_2, \ldots, h_p > 0$

$$2^{-p}u(x) + \sum_{j=0}^\infty \left(\left[\prod_{k=1}^{p}(-1)^{j_k}\delta(k, j_k)\right]F(x)\right)$$

$$= \frac{(-i)^p 2}{(2\pi)^p}h_1\ldots h_p\left[\sum_{v_1=0}^\infty\sum_{v_2=-\infty}^\infty\cdots\sum_{v_p=-\infty}^\infty\text{Re}\left[\frac{\phi(b)e^{-ix'b}}{b_1 b_2\ldots b_p}\right]\right],$$

if p is even, and

$$= -\frac{(-i)^{p-1}2}{(2\pi)^p} h_1 \ldots h_p \left[\sum_{v_1=0}^{\infty} \sum_{v_2=-\infty}^{\infty} \cdots \sum_{v_p=-\infty}^{\infty} \mathrm{Im}\left[\frac{\phi(b)e^{-ix'b}}{b_1 b_2 \ldots b_p} \right] \right], \text{ if } p \text{ is odd,}$$

where $b = (h_1(\frac{1}{2}+v_1), h_2(\frac{1}{2}+v_2), \ldots, h_p(\frac{1}{2}+v_p))' = (b_1, b_2, \ldots, b_p)'.$

6. EXAMPLES OF THE USE OF THE BIVARIATE PROCEDURE

Consider the joint distribution function of the first two non-circular serial correlation coefficients. We follow Durbin's (1980) definition of $r_j = y'A_j y/y'y$ for $j = 1, 2$, as the serial correlation coefficients, where A_1 and A_2 are given below

$$2.A_1 = \begin{bmatrix} 110 & \cdots & 0 \\ 101 & \cdots & 0 \\ 010 & \cdots & 0 \\ \vdots\vdots\vdots & & \vdots\vdots \\ 000 & & 11 \end{bmatrix} \quad \text{and} \quad A_2 = 2.A_1^2 - I, \text{ as } \cos 2\theta = 2\cos^2\theta - 1.$$

For the sake of simplicity we allow y to be a $T \times 1$ vector, containing independent and identically distributed zero mean Gaussian variables.

The eigenvalues of A_j are $\mu_{r_j} = \cos[j\pi(r-1)/T]$, $(r = 1, \ldots, T)$, while they share the same eigenvectors (see Anderson (1971, pp. 282–290)). This means that we can write

$$\Pr(r_1 \le d_1, r_2 \le d_2) = \Pr\left[\sum_{t=1}^{T} u_t^2(\mu_{r_1} - d_1) \le 0, \ \sum_{t=1}^{T} u_t^2(\mu_{r_2} - d_2) \le 0 \right],$$

where $u_t \sim NID(0, 1)$.

Various joint probabilities for the serial correlation coefficients are given in Table 1. In brackets beneath these probabilities are the number of terms in the two dimensional sum used in their computation. The marginal distribution functions were evaluated using Davies (1980) algorithm, with the corresponding induced error chosen to be negligible.

A simulation experiment was performed to check the accuracy of these calculations. When T was less than 100, one million replications were used in the experiment, while for larger T we slowly reduced the number of replications. The Gaussian white noise variables were generated using the Numerical Algorithms Group (1984) routines G05DDF and G05CBF. The experiment showed that the calculations were accurate to four decimal places in every case.

We can see that there is a surprisingly large probability of observing all the serial correlation coefficients to be positive, and a smaller but non-negligible

Table 1 Exact joint probability for the first two serial correlation coefficients with $d = 1.96/\sqrt{T}$

T	$\Pr(X_1 > d, X_2 \leq -d)$	$\Pr(X_1 \leq -d, X_2 > d)$	$\Pr(X_1 > d, X_2 > d)$	$\Pr(X_1 \leq -d, X_2 \leq -d)$
8	0.00000	0.00001	0.00446	0.00000
	(5209)	(5829)	(5822)	(5350)
16	0.00000	0.00007	0.00389	0.00000
	(1856)	(1338)	(1684)	(1565)
32	0.00000	0.00100	0.00279	0.00000
	(601)	(664)	(640)	(686)
64	0.00007	0.00107	0.00204	0.00004
	(373)	(356)	(374)	(358)
128	0.00020	0.00101	0.00157	0.00014
	(253)	(261)	(234)	(236)
256	0.00031	0.00092	0.00125	0.00023
	(209)	(214)	(214)	(211)
512	0.00040	0.00085	0.00105	0.00033
	(201)	(181)	(199)	(203)
1024	0.00047	0.00079	0.00092	0.00041
	(248)	(246)	(246)	(248)
2048	0.00054	0.00077	0.00085	0.00049
	(434)	(432)	(440)	(434)
∞	0.00062	0.00062	0.00062	0.00062

Note: The asymptotic result is calculated using large sample theory.

probability that they alternate in sign—starting with r_1 being negative. This is rather worrying as these patterns are usually taken to indicate the presence of an AR(1) process.

Three other examples of the use of the bivariate inversion theorem exist. The first is by Shively (1988) in tackling a problem in time series econometrics and the second is by Shephard (1990a) in testing for linear restrictions in two different regression models. Finally, by using this technique Shephard (1990b) derives the distribution function of the maximum likelihood estimator of a noninvertible first order moving average.

7. CONCLUSION

In this paper we have developed Riemann sum rules for the inversion of characteristic functions in order to evaluate the distribution function. Although the use of Riemann sums is at first sight primitive, the selection of this technique allows the automatic choice of step sizes. In practice this means that the user only has to be concerned with the issue of truncating the infinite sums at a sensible point. As a result, the suggested rules should be easy to apply in many cases.

In practice these techniques will be used when the characteristic function is cheap to evaluate and the dimension of the integration is reasonably small (less

than five). In these cases there are possibilities of large computational economies when compared with simulation experimentation techniques.

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MATHEMATICAL APPENDIX

Proof of Theorem 1

$$\Pr(X \leq x - t) - \Pr(X > x + t) = -\frac{2}{2\pi} \int_0^\infty \cos[yt] \left(\Delta_y \left[\frac{\phi(y)e^{-iyx}}{yi} \right] \right) dy.$$

Thus

$$\sum_{j=0}^\infty \cos[2\pi zj][\delta(1, j) \Pr(X \leq x)] = F(x) + \sum_{j=1}^\infty \cos[2\pi zj][\delta(1, j) \Pr(X \leq x)]$$

$$= \frac{1}{2} - \frac{1}{2\pi} \sum_{j=-\infty}^{\infty} \exp[-2\pi i j z] \int_0^{\infty} \cos[2\pi j y] \left(\Delta_y \left[\frac{\phi(h_1 y) e^{-ixh_1 y}}{iy} \right] \right) dy.$$

Using Proposition 1

$$= \frac{1}{2} - \frac{1}{2} \frac{1}{2\pi} \sum_{v=-\infty}^{\infty} \left(\Delta_z \left[\frac{\phi(h_1(z+v)) \exp[-ixh_1(z+v)]}{(z+v)i} \right] \right)$$

$$= \frac{1}{2} - \frac{1}{2} \frac{1}{2\pi} \cdot \Delta_z \left[\frac{\phi(h_1 z) \exp[-ixh_1 z]}{zi} \right]$$

$$- \frac{1}{2} \frac{1}{2\pi} \sum_{v=1}^{\infty} \left(\Delta_z \cdot \Delta_{z+v} \left[\frac{\phi(h_1(z+v)) \exp[-ixh_1(z+v)]}{(z+v)i} \right] \right)$$

$$= \frac{1}{2} - \frac{1}{2\pi} \operatorname{Im} \left[\frac{\phi(h_1 z) \exp[-ixh_1 z]}{z} \right]$$

$$- \frac{1}{2\pi} \sum_{v=1}^{\infty} \left(\Delta_z \operatorname{Im} \left[\frac{\phi(h_1(z+v)) \exp[-ixh_1(z+v)]}{(z+v)} \right] \right). \quad \blacksquare$$

Proof of Theorem 2

$$\Pr(X_1 \leqq x_1 - t_1, X_2 \leqq x_2 - t_2) - \Pr(X_1 \leqq x_1 - t_1, X_2 > x_2 + t_2)$$

$$- \Pr(X_1 > x_1 + t_1, X_2 \leqq x_2 - t_2) + \Pr(X_1 > x_1 + t_1, X_2 > x_2 + t_2)$$

$$= \frac{(-2)^2}{(2\pi)^2} \int_0^{\infty} \int_0^{\infty} (\cos[t_1 y_1] \cos[t_2 y_2]) \left(\Delta_{y_1} \cdot \Delta_{y_2} \left[\frac{\phi(y) e^{-ix'y}}{iy_1 iy_2} \right] \right) dy_1 \, dy_2.$$

Hence

$$2^{-2} u(x_1, x_2) + \sum_{j=0}^{\infty} (\cos[2\pi z_1 j_1] \cos[2\pi z_2 j_2]) \delta(1, j_1) \cdot \delta(2, j_2) F(x_1, x_2)$$

$$= \frac{1}{(2\pi)^2} \sum_{j_1=-\infty}^{\infty} \sum_{j_2=-\infty}^{\infty} \exp[-2\pi i[j_1 z_1 + j_2 z_2]]$$

$$\times \int_0^{\infty} \int_0^{\infty} \left(\cos\left[\frac{2\pi j_1}{h_1} \cdot y_1 \right] \cdot \cos\left[\frac{2\pi j_2}{h_2} \cdot y_2 \right] \right)$$

$$\times \left(\Delta_{y_1} \cdot \Delta_{y_2} \left[\frac{\phi(h_1 y_1, h_2 y_2) e^{-ix'(h_1 y_1, h_2 y_2)'}}{ih_1 y_1 \cdot ih_2 y_2} \right] \right) dy_1 \cdot dy_2.$$

So, using Proposition 1, we have for $p = 2$

$$= \frac{1}{(2\pi)^2} \cdot \frac{1}{(2)^2} h_1 h_2 \sum_{v_1 = -\infty}^{\infty} \sum_{v_2 = -\infty}^{\infty} \left(\Delta_{z_1} \cdot \Delta_{z_2} \left[\frac{\phi(a) e^{-ix'a}}{ia_1 ia_2} \right] \right)$$

$$= \frac{1}{(2\pi)^2} \cdot \frac{1}{(2)^2} h_1 h_2 \left[\sum_{v_2 = -\infty}^{\infty} \left(\Delta_{z_2} \cdot \Delta_{z_1} \left[\frac{\phi(h_1 z_1, a_2) e^{-ix'(h_1 z_1, a_2)'}}{ih_1 z_1 ia_2} \right] \right) \right.$$

$$\left. + \sum_{v_1 = 1}^{\infty} \sum_{v_2 = -\infty}^{\infty} \left(\Delta_{z_1} \cdot \Delta_{z_2} \cdot \Delta_{a_1} \left[\frac{\phi(a) e^{-ix'a}}{ia_1 ia_2} \right] \right) \right].$$

Thus

$$2^{-2} u(x_1, x_2) + \sum_{j=0}^{\infty} (\cos[2\pi z_1 j_1] \cos[2\pi z_2 j_2]) \delta(1, j_1) \cdot \delta(2, j_2) F(x_1, x_2)$$

$$= \frac{-1/2}{(2\pi)^2} \cdot h_1 \cdot h_2 \cdot \left[\sum_{v_2 = -\infty}^{\infty} \left(\Delta_{z_2} \operatorname{Re}\left[\frac{\phi(h_1 z_1, a_2) e^{-ix'(h_1 z_1, a_2)'}}{h_1 z_1 a_2} \right] \right) \right.$$

$$\left. + \sum_{v_1 = 1}^{\infty} \sum_{v_2 = -\infty}^{\infty} \left(\Delta_{z_1} \cdot \Delta_{z_2} \operatorname{Re}\left[\frac{\phi(a) e^{-ix'a}}{a_1 a_2} \right] \right) \right]. \quad \blacksquare$$

PROPOSITION 1   *Assume* $\Delta_{z_1} \cdots \Delta_{z_p} g(z_1, \dots, z_p) \in L^p$ *and is both continuous and bounded. Then*

$$\sum_{v_1 = -\infty}^{\infty} \cdots \sum_{v_p = -\infty}^{\infty} (\Delta_{z_1} \cdots \Delta_{z_p} g(v_1 + z_1, \dots, v_p + z_p)) = 2^p \sum_{n_1 = -\infty}^{\infty} \cdots \sum_{n_p = -\infty}^{\infty} e^{-2\pi i n' z} \int_0^{\infty} \cdots \int_0^{\infty}$$

$$\times \left(\prod_{j=1}^{p} \cos[2\pi n_j y_j] \right) (\Delta_{y_1} \cdots \Delta_{y_p} g(y_1, \dots y_p)) dy_1 \dots dy_p,$$

where $n = (n_1, \dots, n_p)'$ *and* $z = (z_1, \dots, z_p)'.$

Proof of Proposition 1   Trivial variant of Poisson's formula, cf. Bohmann (1961) or Zygmund (1955, p. 37).