The Annals of Statistics
1979, Vol. 7, No. 4, 903–910

CALCULATION OF UNIVARIATE AND BIVARIATE NORMAL PROBABILITY FUNCTIONS

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Mill's ratio is expressed as a convergent series in orthogonal polynomials. Truncation of the series provides an approximation for the complemented normal distribution function $Q(x)$, with its maximum error at a finite value of x. The analogous approximation for $xQ(x)$ is used to obtain a new method of calculating the bivariate normal probability function.

1. The univariate normal distribution function. The normal distribution occupies a central position in statistical theory. Many different expressions are available for the univariate normal distribution function. These are of four types: convergent series, continued fractions, asymptotic series, and empirical approximations. The classical formulae have been brought together by Zelen and Severo (1964). Only convergent series are convenient for theoretical work requiring integration of the distribution function. Recently Kerridge and Cook (1976) have derived a new convergent series. Denoting the standard normal probability density by

$$Z(y) \equiv (2\pi)^{-\frac{1}{2}} \exp(-y^2/2);$$

their result is

$$\int_0^x Z(y)\, dy = (2\pi)^{-\frac{1}{2}} x e^{-x^2/8} \sum_{n=0}^{\infty} \theta_{2n}(x/2)/(2n+1)$$

where θ_n is related to the Hermite polynomial H_n through the equation

$$\theta_n(y) = y^n H_n(y)/n!$$

and therefore

$$\theta_{n+1}(y) = y^2[\theta_n(y) - \theta_{n-1}(y)]/(n+1).$$

While this series converges more rapidly than previous ones, its convergence becomes slower as x increases. Therefore it cannot be used to approximate the distribution function in an integrand.

What is needed is a series with its maximum error at some finite value of x. Let us use an nth degree polynomial to approximate Mill's ratio $Q(x)/Z(x)$ where

$$Q(x) = \int_x^\infty Z(y)\, dy.$$

Received February 1977; revised November 1977.

AMS 1970 *subject classifications.* Primary 60E05; secondary 41A10.

Key words and phrases. Univariate normal probability, bivariate normal probability, polynomial approximation, orthogonal polynomials.

Let

$$(1.1) \qquad Q(x)/Z(x) \cong \Sigma_{k=0}^{n} a_{nk} x^k \qquad x \geqslant 0.$$

We choose the coefficients so as to minimize the integral

$$\int_0^\infty \left[Q(x) - Z(x) \Sigma_{k=0}^{n} a_{nk} x^k \right]^2 dx$$
$$= (2\pi)^{-1} \int_0^\infty \left[Q(x)/Z(x) - \Sigma_{k=0}^{n} a_{nk} x^k \right]^2 e^{-x^2} dx.$$

It is well known that the polynomial which minimizes this integral is equal to $\Sigma_{k=0}^{n} b_k p_k(x)$ where $p_k(x)$ is the kth degree polynomial belonging to an orthonormal set:

$$(1.2) \qquad \int_0^\infty p_j(x) p_k(x) e^{-x^2} dx = \delta_{jk}$$

and

$$(1.3) \qquad b_k = \int_0^\infty \left[Q(x)/Z(x) \right] p_k(x) e^{-x^2} dx.$$

(See, e.g., Szegö (1959).)

Let

$$p_k(x) = \Sigma_{j=0}^{k} c_{kj} x^j.$$

There does not seem to be any simple formula or recurrence relation for the c_{kj}. The complexity of the polynomials becomes evident if one seeks a Rodrigues-type expression of the form

$$e^{-x^2} p_k(x) = d^k F_k(x)/dx^k.$$

Integration by parts shows that, in order to satisfy

$$\int_0^\infty x^j P_k(x) e^{-x^2} dx = 0, \qquad j = 0, 1, \cdots, (k-1),$$

$F_k(x)$ and its first $(k-1)$ derivatives must vanish at $x = 0$. The required function is of the form

$$F_k(x) = \Sigma_{j=0}^{k} \alpha_{kj} E_j(x)$$

where $E_0(x) = e^{-x^2}$ and

$$E_j(x) = \int_x^\infty E_{j-1}(y)\, dy \qquad j > 0.$$

The conditions at $x = 0$ yield k simultaneous equations for the α's.

The coefficients c_{kj} can be found by Schmidt orthogonalization, starting with $k = 0$. The inner products needed for this purpose are given by

$$(1.4) \qquad (x^i, x^j) = \int_0^\infty x^i x^j e^{-x^2} dx$$
$$\equiv I_{i+j}.$$

It is easy to show that

$$I_0 = (\pi)^{\frac{1}{2}}/2,$$
$$I_1 = \tfrac{1}{2},$$

and

$$I_k = (k-1)I_{k-2}/2 \qquad k \geqslant 2.$$

The coefficients b_k are then given by

$$(1.5) \qquad b_k = (2\pi)^{\frac{1}{2}} \int_0^\infty Q(x) e^{-x^2/2} p_k(x)\, dx$$
$$= \Sigma_{j=0}^k c_{kj} (2\pi)^{\frac{1}{2}} \int_0^\infty Q(x) e^{-x^2/2} x^j\, dx.$$

The quantity multiplying c_{kj} in this sum is

$$J_j \equiv (2\pi)^{\frac{1}{2}} \int_0^\infty x^j e^{-x^2/2}\, dx \int_x^\infty (2\pi)^{-\frac{1}{2}} e^{-y^2/2}\, dy.$$

The region of integration is $y \geqslant x \geqslant 0$. Therefore, with $r = (x^2 + y^2)^{\frac{1}{2}}$ and $\varphi = \arctan(y/x)$,

$$(1.6) \qquad J_j = \int_0^\infty r^{j+1} e^{-r^2/2}\, dr \int_{\pi/4}^{\pi/2} (\cos \varphi)^j\, d\varphi.$$

Integration by parts yields simple recurrence relations for the integrals over r and φ.

Thus we arrive at the following least squares approximation for $Q(x)$.

$$Q(x) \cong Z(x) \Sigma_{j=0}^n a_{nj} x^j \qquad x \geqslant 0$$

where

$$(1.7) \qquad a_{nj} = \Sigma_{k=j}^n c_{kj} b_k$$
$$= \Sigma_{k=j}^n c_{kj} \Sigma_{i=0}^k c_{ki} J_i.$$

The coefficients were evaluated using a digital computer. It was found that a series with $n = 10$ had a maximum absolute error less than 3×10^{-7}. The maximum error decreased roughly by a factor of 4 with each additional term. The error curve on using a polynomial of degree n has $(n + 1)$ extrema with extreme values alternating in sign. The error tends to zero when $x \to \infty$. For any given ε one can determine a value of n which makes the maximum absolute error less than ε. Then the approximation will have the desired accuracy for all $x \geqslant 0$. This makes a series of this type very useful in theoretical work, as illustrated in the next section.

For $n = 10$ the coefficients a_{nj} to ten significant digits are as follows. (The redundant subscript $n = 10$ has been omitted.)

$$a_0 = 1.2533\,13402 \qquad a_1 = -0.99996\,73043$$
$$a_2 = 0.62629\,72801 \qquad a_3 = -0.3316218430$$
$$a_4 = 0.15227\,23563 \qquad a_5 = -5.9828\,34993 \times 10^{-2}$$
$$a_6 = 1.9156\,49350 \times 10^{-2} \qquad a_7 = -4.6449\,60579 \times 10^{-3}$$
$$a_8 = 7.7710\,88713 \times 10^{-4} \qquad a_9 = -7.8308\,23677 \times 10^{-5}$$
$$a_{10} = 3.5342\,44658 \times 10^{-6}$$

2. The bivariate normal probability function. The bivariate normal probability function is defined by

$$L(h, k; \rho) \equiv \int_h^\infty \int_k^\infty f(x, y; \rho)\, dy\, dx \tag{2.1}$$

where

$$f(x, y; \rho) \equiv \frac{(2\pi)^{-1}}{(1-\rho^2)^{\frac{1}{2}}} \exp\left[-(x^2 + y^2 - 2xy\rho)/2(1-\rho^2)\right]. \tag{2.2}$$

Various methods have been proposed for approximate evaluation of the function L. These have been reviewed by Gupta (1963). The approach which has attracted the most attention in recent years is that of Owen (1956). He expressed the bivariate probability in terms of the univariate distribution function and the function T defined by

$$T(h, a) = (2\pi)^{-1} \int_0^a \exp\left[-h^2(1 + y^2)/2\right] dy/(1 + y^2). \tag{2.3}$$

If x' and y' are independent standard normal variables and $a \geqslant 0$, $T(h, a)$ equals the probability in the region

$$x' \geqslant h; \qquad ax' \geqslant y' \geqslant 0.$$

Owen evaluated the integral in equation (2.3) by expanding the exponential in a power series and integrating term by term.

Recent papers by Borth (1973), Daley (1974), and Young and Minder (1974) have all concentrated on more efficient computation of Owen's T function. While the others evaluate the integral by quadrature, Borth uses a Chebyshev approximation for $1/(1 + y^2)$ when $h > 1.6$ and $a > 0.3$. This reduces the computation required for given accuracy because Owen's series converges slowly when both h and a are large.

It is possible to obtain a more efficient procedure by using a different reduction of $L(h, k; \rho)$ to functions of one and two arguments. Let $x' = x$ and

$$y' = (k - \rho x)/(1 - \rho^2)^{\frac{1}{2}}.$$

Then x' and y' are independent standard normal variables. The lines $x = h$ and

$y = k$ are mapped into $x' = h$ and

$$y' = (k - \rho x')/(1 - \rho^2)^{\frac{1}{2}}$$

respectively. Their point of intersection is (h', k') where $h' = h$ and

$$k' = (k - \rho h)/(1 - \rho^2)^{\frac{1}{2}}.$$

The polar coordinates (R', θ) of $(h', k') \neq (0, 0)$ are given by

$$R'^2 = (h^2 + k^2 - 2hk\rho)/(1 - \rho^2)$$

$$\sin(\pi/2 - \theta) = h/R'$$

and

$$\cos(\pi/2 - \theta) = (k - \rho h)/\left[R'(1 - \rho^2)^{\frac{1}{2}}\right].$$

$L(h, k; \rho)$ equals the probability in the region

$$x' \geqslant h'; \qquad y' \geqslant k' + \rho(h' - x')/(1 - \rho^2)^{\frac{1}{2}}. \tag{2.4}$$

The angle from the x' axis to the boundary defined by the second inequality will be denoted by φ. (See Figure 1, where the value of φ is negative.)

$$\tan \varphi = -\rho/(1 - \rho^2)^{\frac{1}{2}}.$$

Therefore

$$\sin(\theta - \varphi) = k/R'$$

and

$$\cos(\theta - \varphi) = (h - \rho k)/\left[R'(1 - \rho^2)^{\frac{1}{2}}\right].$$

The angles $(\pi/2 - \theta)$ and $(\theta - \varphi)$ are taken to lie in $(-\pi, \pi]$. If $h' = k' = 0$,

$$\tan(\pi/2 - \theta) = \tan(\theta - \varphi) = \left[(1 + \rho)/(1 - \rho)\right]^{\frac{1}{2}}.$$

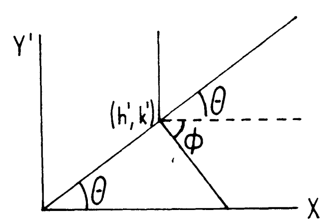

FIG. 1. *Angles used in Equation* (2.7).

The probability in the region defined by the inequalities (2.4) can be expressed in terms of a modification of the W function introduced by Ruben (1961). For $\pi \geqslant \psi \geqslant 0$, the function $W(R, \psi)$ is defined as the probability in the sector

$$x' \geqslant R; \qquad (x' - R)\tan \psi \geqslant y' \geqslant 0.$$

(See Figure 2.) As x' and y' are independent, the probability density in the (x', y')

plane is circularly symmetric. Therefore the probability in the sector does not change if the sector is rotated about the origin. For $\psi < 0$ we define the function by

$$W(R, \psi) = -W(R, |\psi|). \tag{2.5}$$

This part of the definition differs from Ruben's, and leads to simpler formulae. From Figure 2 we see that when $\psi \geqslant 0$,

$$W(R, \psi) + W(R, \pi - \psi) = Q(R \sin \psi). \tag{2.6}$$

The desired probability is given by

$$L(h, k; \rho) = W(R', \pi/2 - \theta) + W(R', \theta - \varphi) + C \tag{2.7}$$

where $C = 1$ if $h < 0$, $k < 0$; and $C = 0$ otherwise. In the former case, the origin lies inside the region of integration.

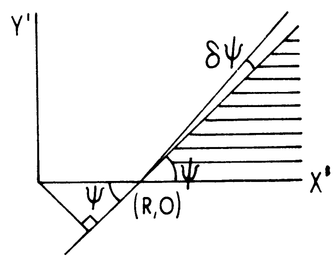

FIG. 2. *Region of integration for $W(R, \psi)$.*

$[\partial W(R, \psi)/\partial\psi]\delta\psi$ is the probability in the infinitesimal triangular wedge with apex at $(R, 0)$ and boundaries making angles ψ and $\psi + \delta\psi$ with the x' axis. Let s be the distance of a point in the wedge from $(R, 0)$. Then

$$\partial W(R, \psi)/\partial\psi = (2\pi)^{-1}\textstyle\int_0^\infty e^{-r'^2/2} s\, ds \tag{2.8}$$

where

$$r'^2 = x'^2 + y'^2 = R^2 + s^2 + 2Rs \cos \psi.$$

After changing the variable of integration to $s' = s + R \cos \psi$ one obtains

$$\partial W(R, \psi)/\partial\psi = e^{-R^2/2}/2\pi - (2\pi)^{-1}e^{-R^2 \sin^2 \psi/2}(2\pi)^{\frac{1}{2}} R \cos \psi Q(R \cos \psi); \tag{2.9}$$

$W(R, \psi)$ is the integral of the right hand side from 0 to ψ. Ruben (1961) gave a continued fraction for the function

$$K(R, \psi) = \psi e^{-R^2/2}/2\pi - W(R, \psi).$$

As the continued fraction was not suitable for practical computations, the W function seemed to be of academic interest only. However, it is possible to approximate the second term on the right in equation (2.9) with a series analogous to that in Section 1. We write

$$xQ(x) \cong xZ(x)\Sigma_{k=0}^n d_{nk} x^k \qquad x \geqslant 0 \tag{2.10}$$

and minimize

$$\int_0^\infty \left[xQ(x) - xZ(x)\Sigma_{k=0}^n d_{nk}x^k\right]^2 dx$$
$$= (2\pi)^{-1}\int_0^\infty \left[Q(x)/Z(x) - \Sigma_{k=0}^n d_{nk}x^k\right]^2 (x^2 e^{-x^2})\, dx.$$

The problem is similar to that in Section 1 with the weight function $x^2e^{-x^2}$ instead of e^{-x^2}. The orthogonal polynomials and then the coefficients d_{nk} can be calculated using the same families of integrals, I_m and J_m.

A series of 11 terms was again found adequate for an accuracy of the order of 10^{-7}. A maximum absolute error of 1.24×10^{-7} in $xQ(x)$ was obtained with the approximation

$$xQ(x)/Z(x) \cong x\Sigma_{k=0}^{10} d_k x^k \qquad x \geqslant 0 \tag{2.11}$$

where

$$\begin{aligned}
d_0 &= 1.2532\,98042 & d_1 &= -0.99973\,16607\\
d_2 &= 0.62501\,92459 & d_3 &= -0.32819\,15667\\
d_4 &= 0.14703\,31965 & d_5 &= -5.4948\,56177 \times 10^{-2}\\
d_6 &= 1.6298\,27794 \times 10^{-2} & d_7 &= -3.5912\,57830 \times 10^{-3}\\
d_8 &= 5.4066\,19903 \times 10^{-4} & d_9 &= -4.8902\,54061 \times 10^{-5}
\end{aligned}$$

$$d_{10} = 1.9847\,41031 \times 10^{-6}.$$

When we use this approximation in the integrand for $W(R, \psi)$ given by equation (2.9), the error in the integrand will not exceed $1.24 \times 10^{-7}/(2\pi)^{\frac{1}{2}}$. We have

$$\partial W(R, \psi)/\partial\psi \cong e^{-R^2/2}/2\pi - (2\pi)^{-1}e^{-R^2\sin^2\psi/2}R\cos\psi e^{-R^2\cos^2\psi/2}$$
$$\times \Sigma_{k=0}^{10} d_k (R\cos\psi)^k \qquad \cos\psi \geqslant 0.$$

Therefore

$$W(R, \psi) \cong (2\pi)^{-1}e^{-R^2/2}\left[\psi - \Sigma_{k=0}^{10} d_k R^{k+1}\int_0^\psi (\cos\psi')^{k+1}\, d\psi'\right] \qquad |\psi| \leqslant \pi/2. \tag{2.12}$$

Equations (2.12), (2.5) and (2.6) together suffice for all calculations.

We now have a new method for calculating the bivariate normal probability function $L(h, k; \rho)$. One can reduce the error by using more terms in the polynomial in equation (2.10). Limitations on accuracy arise only from roundoff errors in computation of the coefficients d_{nk}. The present algorithm was coded as a Fortran subroutine using single precision arithmetic on an IBM 370/155 computer. Accuracy was checked by comparison with a similar subroutine using $n = 12$ and double precision arithmetic. The new algorithm was found to be more accurate and considerably faster than the Owen–Borth algorithm.

Acknowledgment. It is a pleasure to thank Mr. K. V. Subba Rao for helpful discussions and his careful reading of the manuscript.

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