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ABSTRACT

The probability integral of the multivariate normal distribution (ND) has received considerable attention since W. F. Sheppard's (1900) and K. Pearson's (1901) seminal work on the bivariate ND. This paper evaluates the formula that represents the "n x n" correlation matrix of the "chi(sub i)" and the standardized multivariate normal density function. C. W. Dunnett and M. Sobel's formula for the univariate ND function, and R. E. Bohrer and M. J. Schervish's error-bounded algorithm for evaluating "F(sub n)" for general "rho(sub ij)" are discussed. Computationally, the latter algorithm is restricted to "n = 7"; even at "n = 7", it can take up to 24 hours for it to compute a single probability with 10(sup -3) accuracy on a computer than is capable of about 1-2 million scalar floating point operations/second. This report presents a fast and general approximation (APX) for rectangular regions of the multivariate ND function based on C. E. Clark's (1961) APX to the moments of the maximum of "n" jointly normal random variables. The performance of this APX compared to special cases in which the exact results are known and error-bounded reduction formulae show that the APX's accuracy is adequate for many practical applications where multivariate normal probabilities are required. The computational speed of the Clark APX is unparalleled. The error bound for the APX is about 10(sup -3) regardless of dimensionality, and accuracy increases with increases in "rho". The Clark algorithm provides a generalization of Dunnett's (1955) results to the case of general "rho(sub ij)", a natural application of which would be a generalization of Dunnett's test to the case of unequal sample sizes among the "k + 1" groups (i.e., multiple treatment groups compared to a single control group). One data table is included. (RLC)

Approximating Multivariate Normal Orthant Probabilities

ONR Technical Report

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$$F_n(h_1, h_2, \ldots, h_n; \{\rho_{ij}\}) = \int_{-\infty}^{h_1}\int_{-\infty}^{h_2}\cdots\int_{-\infty}^{h_n} f(x_1, x_2, \ldots, x_n; \{\rho_{ij}\})dx_1 \ldots dx_n$$

where $\{\rho_{ij}\}$ represents the n x n symmetric correlation matrix of the x_i's, and $f(x_1, x_2, \ldots, x_n; \{\rho_{ij}\})$ is the standardized multivariate normal density function. Direct evaluation of F_n is only possible for special cases of $\{\rho_{ij}\}$. For example, Dunnett and Sobel (1955) have shown that when $\rho_{ij} = \alpha_i\alpha_j (i \neq j)$, where $|\alpha_i| \leq 1$, then

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$$F_n(h_1, h_2, \ldots, h_n; \{\rho_{ij}\}) = \int_{-\infty}^{\infty} \left[\prod_{i=1}^{n} \Phi \left(\frac{h_i - \alpha_i y}{\sqrt{1 - \alpha^2}} \right) \right] f(y) d(y)$$

where Φ represents the univariate normal distribution function. This special case is the basis for much of item-response theory. More recently, however, Bohrer and Schervish (1981), have developed an error bounded algorithm for evaluating F_n for general $\{\rho_{ij}\}$. Computationally, this algorithm is restricted to $n = 7$, and even at $n = 7$, it can require as much as 24 hours to compute a single probability with 10^{-3} accuracy on a computer than is capable of approximately 1-2 million scalar floating point operations per second.

The purpose of this report is to present a fast and general approximation for rectangular regions of the multivariate normal distribution function, that is based on Clark's (1961) approximation to the moments of the maximum of n jointly normal random variables. The performance of this approximation is then compared to special cases in which the exact results are known (*e.g.*, $\rho_{ij} = \rho = .5$), cases in which the integral reduces to a unidimensional quadrature evaluation (*e.g.*, $\rho_{ij} = \alpha_i \alpha_j$), and finally error bounded reduction formulae for $\{\rho_{ij}\}$ and $n \leq 7$.

ABSTRACT

The probability integral of the multivariate normal distribution has received considerable attention since Sheppard (1900) and Pearson (1901) published their seminal work on the bivariate normal distribution. In the general case, we are concerned with evaluating

$$F_n(h_1, h_2, \ldots, h_n; \{\rho_{ij}\}) = \int_{-\infty}^{h_1}\int_{-\infty}^{h_2}\cdots\int_{-\infty}^{h_n} f(x_1, x_2, \ldots, x_n; \{\rho_{ij}\})dx_1 \ldots dx_n$$

where $\{\rho_{ij}\}$ represents the n x n correlation matrix of the x_i's, and $f(x_1, x_2, \ldots, x_n; \{\rho_{ij}\})$ is the standardized multivariate normal density function. Direct evaluation of F_n is only possible for special cases of $\{\rho_{ij}\}$. For example, Dunnett and Sobel (1955) have shown that when $\rho_{ij} = \alpha_i\alpha_j (i \neq j)$, where $| \alpha_i | \leq 1$, then

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where Φ represents the univariate normal distribution function. This special case is the basis for much of modern psychometric theory. More recently, however, Bohrer and Schervish (1981), have developed an error-bounded algorithm for evaluating F_n for general $\{\rho_{ij}\}$. Computationally, this algorithm is restricted to $n = 7$, and even at $n = 7$, it can require as much as 24 hours to compute a single probability with 10^{-3} accuracy on a computer than is capable of approximately 1-2 million scalar floating point operations per second.

The purpose of this report is to present a fast and general approximation for rectangular regions of the multivariate normal distribution function based on Clark's (1961) approximation to the moments of the maximum of n jointly normal random variables. The performance of this approximation compared to special cases in which the exact results are known and error-bounded reduction formulae show the accuracy of the approximation to be adequate for many practical applications where multivariate normal probabilities are required.

1 Introduction

The probability integral of the multivariate normal distribution has received considerable attention since Sheppard (1900) and Pearson (1901) published their seminal work on the bivariate normal distribution. In the general case, we are concerned with evaluating

$$F_n(h_1, h_2, \ldots, h_n; \{\rho_{ij}\}) = \int_{-\infty}^{h_1} \int_{-\infty}^{h_2} \cdots \int_{-\infty}^{h_n} f(x_1, x_2, \ldots, x_n; \{\rho_{ij}\}) dx_1 \ldots dx_n \tag{1}$$

where $\{\rho_{ij}\}$ represents the n x n symmetric correlation matrix of the x_i's, and $f(x_1, x_2, \ldots, x_n; \{\rho_{ij}\})$ is the standardized multivariate normal density function. Direct evaluation of F_n is only possible for special cases of $\{\rho_{ij}\}$. For example. Dunnett and Sobel (1955) have shown that when $\rho_{ij} = \alpha_i\alpha_j (i \neq j)$. where $| \alpha_i | \leq 1$. then

$$F_n(h_1, h_2, \ldots, h_n; \{\rho_{ij}\}) = \int_{-\infty}^{\infty} \left[\prod_{i=1}^{n} \Phi \left(\frac{h_i - \alpha_i y}{\sqrt{1 - \alpha^2}} \right) \right] f(y) d(y) \tag{2}$$

where Φ represents the univariate normal distribution function. The probability in equation (2) can be approximated to any practical degree of accuracy using Gauss-Hermite quadrature (Stroud and Sechrest, 1966). It should be noted that when $\rho_{ij} = \rho$ for all i, j, then

$$F_n(h, h, \ldots, h; \{\rho\}) = \int_{-\infty}^{\infty} \left[\Phi^n \left(\frac{h + \rho^{1/2} y}{\sqrt{1 - \rho}} \right) \right] f(y) d(y) \tag{3}$$

and if $\rho = .5$ and $h = 0$.

$$F_n(0, 0, \ldots, 0; \{.5\}) = \frac{1}{n + 1} \tag{4}$$

More recently, however, Bohrer and Schervish (1981), have developed an error-bounded algorithm for evaluating F_n for general $\{\rho_{ij}\}$. Computationally, this algorithm is restricted to $n = 7$, and even at $n = 7$, it can require as much as 24 hours to compute a single probability with 10^{-2} accuracy on a computer than is capable of approximately 1-2 million scalar floating point operations per second. It is unclear whether vectorization of this algorithm is possible, so that the greatly increased speeds of parallel computing environments could be exploited (*e.g.*, 20-80 million floating point instructions per second). Even still, it is unlikely that this algorithm would be computational tractable for $n > 10$.

An alternate approach to approximating F_n, can be obtained by noting that

$$F_n = Pr(x_1 \le h_1, x_2 \le h_2, \ldots x_n \le h_n) \tag{5}$$

If $h_1 \ldots h_n = h = 0$. and the x_i follow a standardized multivariate normal distribution. F_n^0 is a so-called "orthant" probability. Note, however. that this orthant probability is equivalent to

$$F_n^0 = Pr\{max(x_1, \ldots, x_n) \le 0\} \tag{6}$$

If $max(x_1, \ldots, x_n)$ were normally distributed. which it clearly is not, with mean $E[max(x_1, \ldots, x_n)]$ and variance $V[max(x_1, \ldots, x_n)]$, then,

$$F_n^0 = \Phi\left[\frac{h - E(max(x_1, \ldots, x_n)}{\sqrt{V(max(x_1, \ldots, x_n)}}\right] \tag{7}$$

where in this case $h = 0$. For the more general rectangular region case of h_i, we could set $h = 0$ and subtract h_i from the mean values of each of the x_i, which to this point have been expressed in standardized form.

To use this algorithm. we must first have an accurate method of computing the first two moments of $max(x_1, \ldots x_n)$ where the x_i have a joint multivariate normal distribution with general correlation $\{\rho_{ij}\}$, and some bound on the error introduced by assuming that $max(x_1, \ldots x_n)$ has a normal distribution. Such an approximation has been described by Clark (1961), and in the following, we describe its use in connection with evaluating $F_n(x_1, x_2, \ldots, x_n; \{\rho_{ij}\})$. We begin by reviewing Clark's original formulae.

2 The Clark Algorithm

Let any three successive components from an n-variate vector. $\mathbf{y}_i$. be distributed:

$$\begin{bmatrix} y_i \\ y_{i+1} \\ y_{i+2} \end{bmatrix} \sim N\left(\begin{bmatrix} \mu_i \\ \mu_{i+1} \\ \mu_{i+2} \end{bmatrix}, \begin{bmatrix} \sigma_i^2 & & \\ \sigma_i \sigma_{i+1} \rho_{i,i+1} & \sigma_{i+1}^2 & \\ \sigma_i \sigma_{i+2} \rho_{i,i+2} & \sigma_{i+1} \sigma_{i+2} \rho_{i+1,i+2} & \sigma_{i+2}^2 \end{bmatrix}\right)$$

Let $\tilde{y}_i = \max(y_i) = y_i$. and compute the probability that $y_{i+1} > \tilde{y}_i$ as follows:

$$\begin{aligned} \text{set} \qquad z_{i+1} &= (\mu_i - \mu_{i+1})/\zeta_{i+1}, \\ \text{where} \qquad \zeta_{i+1}^2 &= \sigma_i^2 + \sigma_{i+1}^2 - 2\sigma_i \sigma_{i+1} \rho_{i,i+1}. \\ \text{Then} \quad P(y_{i+1} > \tilde{y}) &= P(y_{i+1} - \tilde{y} > 0) \\ &= \Phi(-z_{i+1}) \end{aligned}$$

the value of the univariate normal distribution function at the standard deviate $-z_{i+1}$.

Now let $\tilde{y}_{i+1} = \max(y_i, y_{i+1})$ and assume (as an approximation) that $(y_{i+2}, \tilde{y}_{i+1})$ is bivariate normal with means,

$$\begin{aligned} \mu(y_{i+2}) &= \mathcal{E}(y_{i+2}) = \mu_{i+2} \\ \mu(\tilde{y}_{i+1}) &= \mathcal{E}(\tilde{y}_{i+1}) = \mu_i\Phi(z_{i+1}) + \mu_{i+1}\Phi(-z_{i+1}) + \zeta_{i+1}\phi(z_{i+1}), \end{aligned} \tag{8}$$

variances

$$\begin{aligned} \sigma^2(y_{i+2}) &= \mathcal{E}(y_{i+2}^2) - \mathcal{E}^2(y_{i+2}) = \sigma_{i+2}^2 \\ \sigma^2(\tilde{y}_{i+1}) &= \mathcal{E}(\tilde{y}_{i+1}^2) - \mathcal{E}^2(\tilde{y}_{i+1}) = \sigma_{i+2}^2, \end{aligned} \tag{9}$$

where

$$\mathcal{E}(\tilde{y}_{i+1}^2) = (\mu_i^2 + \sigma_i^2)\Phi(z_{i+1}) + (\mu_{i+1}^2 + \sigma_{i+1}^2)\Phi(-z_{i+1}) + (\mu_i + \mu_{i+1})\zeta_{i+1}\phi(z_{i+1}), \tag{10}$$

and correlation

$$\rho(\tilde{y}_{i+1}, y_{i+2}) = \frac{\sigma_i\rho_{i,i+2}\Phi(z_{i+1}) + \sigma_{i+1}\rho_{i+1,i+2}\Phi(-z_{i+1})}{\sigma(\tilde{y}_{i+1})}. \tag{11}$$

Then,

$$P(y_{i+2} = \max(y_i, y_{i+1}, y_{i+2})) = P((y_{i+2} - y_{i+1} > 0) \cap (y_{i+2} - y_i > 0)) \tag{12}$$

is approximated by

$$\begin{aligned} P(y_{i+2} > \tilde{y}_{i+1}) &= P(y_{i+2} - \tilde{y}_{i+1} > 0) \\ &= \Phi\left(\frac{\mu_{i+2} - \mu(\tilde{y}_{i+1})}{\sqrt{\sigma_{i+2}^2 + \sigma^2(\tilde{y}_{i+1}) - 2\sigma_{i+2}\sigma(\tilde{y}_{i+1})\rho(\tilde{y}_{i+1}, y_{i+2})}}\right) \end{aligned} \tag{13}$$

Assuming as a working approximation that $\tilde{y}_{i+1}$ is normally distributed with the above mean and variance, we may therefore proceed, recursively from $i = 1$ to $i = n - 1$, where y_{n+1} is an independent dummy variate with mean zero and variance zero (i.e. $y_{n+1} = 0$). Then, for example,

$$
\begin{aligned}
&P[y_{n+1} = \max(y_1, y_2, \ldots, y_{n+1})] \\
&\quad = P\left[(y_{n+1} - y_1 > 0) \cap (y_{n+1} - y_2 > 0) \cap \ldots \cap (y_{n+1} - y_n > 0)\right] \\
&\quad = P\left[(-y_1 > 0) \cap (-y_2 > 0) \cap \ldots \cap (-y_n > 0)\right]
\end{aligned} \tag{14}
$$

approximates the probability of the negative orthant of the specified multivariate normal distribution. In the case of n correlated standard normals, the negative and positive orthant probabilities are identical. The probability of any other orthant can be obtained by reversing the signs of the variates corresponding to 1's in the orthant pattern. Of course, $\tilde{y}_{i+1}$ is not normally distributed. Errors produced by substituting normal approximations for the moments of $\tilde{y}_{i+1}$ are discussed in the following section.

More generally, to compute a multivariate normal probability over an n dimensional rectangular region, for example,

$$\int_{-\infty}^{h} \int_{-\infty}^{h} \cdots \int_{-\infty}^{h} f(x_1, x_2, \ldots, x_n; \{\rho_{ij}\}) dx_1 \ldots dx_n \tag{15}$$

we compute the negative orthant setting $\mu_{n+1} = h$. Finally, to approximate the integral for general h_i, we compute the negative orthant by setting $\mu_{n+1} = 0$ and $\mu_i = \mu_i - h_i$.

3 Accuracy of the Clark Approximation

The errors of the Clark approximation result from the replacement of non-normal distributions by normal approximations. For example, suppose that we are interested in the maximum of four standard normal variables, *i.e.*, $max(y_1, y_2, y_3, y_4)$. By assuming that $\tilde{y}_2$ is normally distributed with expected value $E[max(y_1, y_2)]$ and variance $V[max(y_1, y_2)]$, we can then use the moments of $max(\tilde{y}_1, y_3)$ as an approximation for those of $max(y_1, y_2, y_3)$. Next, we assume that $\tilde{y}_3$ is normally distributed with expectation and variance equal to the corresponding moments of $max(\tilde{y}_2, y_3)$, and can therefore use the moments of $max(\tilde{y}_3, y_4)$ as an approximation for those of $max(y_1, \ldots, y_4)$. In this example, of course, $\tilde{y}_2$ and $\tilde{y}_3$ are not normally distributed. Furthermore, this is a rare case in which the distribution of a statistical variate diverges from normality as sample size increases. Tippet (1925) first showed that skewness and kurtosis of the maximum of n standard normals goes form .019 and .62 respectively for $n = 2$ to .429 and .765 for $n = 100$ to .618 and 1.088 for $n = 1000$. In terms of expected values of n standard normal variables, the effect of this non-normality is quite small. For example, for $n = 10$, the true value is

1.5388 and the approximation yields 1.5367. Even for $n = 1000$ the expected value is 3.2414 and the approximated value is 3.2457.

The effect of non-normality on the accuracy of the approximation is also dependent on the difference between $E(\tilde{y}_{i-1}, y_i)$. For example, suppose we wish to approximate the moments of $max(y_1, y_2)$ where y_1 and y_2 are not normally distributed. Clark (1961) points out that if the difference $E(y_1) - E(y_2)$ is large relative to the greater of $V^{1/2}(y_1)$ and $V^{1/2}(y_2)$ the random variable $max(y_1, y_2)$ is almost identical to y_1. Certainly the first two moments of $max(y_1, y_2)$ would be minimally affected by replacing y_1 and y_2 by normal approximations. However if $E(y_1) - E(y_2)$ is small relative to the respective standard deviations, then the use of normal approximations could conceivably result in significant errors in the approximation of the mean and variance of their maximum.

In light of this, the following illustrations of the accuracy of the Clark approximation are, in fact, the worst case results, since they represent the case in which the expected values of the y_i are equal. These results indicate that the error bound for the Clark approximation is approximately 10^{-3}, as illustrated in the following section.

4 Illustration

To evaluate the performance of this algorithm, we have examined a series of equa-correlated multivariate normal distributions for which exact results are known (see Gupta, 1963) and those considered by Schervish (1984). Table 1A displays results for 3 to 7 equa-correlated standard normal random variables with selected values of $\rho = .2, .3, .8$ and .9, and upper integration bounds of 0, 1, and 2. Inspection of the tabled probabilities reveals that the Clark algorithm is generally accurate to at least 10^{-3} and that computational times are a linear function of dimensionality. The speed of the Clark algorithm does not depend on ρ. In contrast, the speed of MULNOR (Schevish, 1984) is exponentially increasing with both dimensionality and ρ. In the 7-variate normal case with $\rho_{ij} = .9$, MULNOR required almost a day to compute a probability which was accurate to 2×10^{-5}, whereas the Clark algorithm computed the same probability with 4×10^{-4} accuracy in less than three thousandths of a second. Inspection of these results and others not reported here, suggest that the accuracy of the Clark approximation increases with increasing ρ.

Table 1B displays results for orthant probabilities of higher dimensional integrals (n = 10, 20, and 40), for the special case of $\rho = .5$, where $F_n^0 = 1/(n+1)$. Again, results are accurate to at least 10^{-3}, and computational times are linear in n. MULNOR could not be used to evaluate integrals of this dimensionality.

Finally, Table 1C displays results for some tail probabilities of the multivariate normal distribution. In this case, the upper bound of the integration was -2.5, $n = (3,5,10)$, and $\rho = (.5,.9)$. These probabilities ranged from 10^{-3} to 10^{-5} and accuracy of the Clark approximation was 10^{-5} in all cases.

5 Discussion

Clark's (1961) formulae for the moments of the maximum of n correlated random normal variates can clearly be used to obtain a fast and accurate approximation to multivariate normal probabilities. Examination of a series of examples involving special cases in which the true results are known, reveals that the error bound for the approximation is approximately 10^{-3} regardless of dimensionality, and that accuracy increases with increases in $\mid \rho \mid$. These results are conservative in that we would expect the ill effect of using normal approximations to be greatest when $\mu_i = \mu, (i = 1, n)$ which is the case used in the illustrations.

In terms of computational speed, the Clark approximation is clearly unparalleled. A reasonable estimate of the speed of the Clark algorithm is given by,

$$\text{speed} = \left(\frac{.0004(n)}{\text{megaflop}} \right) \text{seconds}$$

where megaflop is the number of scalar floating point instructions per second that the computer is capable of performing.

Numerous applications of the Clark algorithm suggest themselves. Some preliminary work in this area has already been conducted by Daganzo (1984), in the context of discrete choice models of consumer behavior, and by Gibbons, Bock and Hedeker (1987) in item-response theory. Other potential applications include multivariate generalizations of probit analysis (see Ashford and Sowden, 1970 for the bivariate case), and random-effect probit models (Gibbons and Bock, 1987), where the Clark approximation was used to estimate first-order autocorrelation among the residual errors.

Another area of potential interest is in the approximation of multivariate t probabilities, which can be considered as the joint distribution of n variates $t_i = z_i/s, (i = 1, 2, \ldots, n)$ where the z_i have a multivariate normal distribution with zero means and unknown variance σ^2, and known correlation matrix $\{\rho_{ij}\}$, while $\nu s^2/\sigma^2$ has a χ^2 distribution with ν degrees of freedom and is independent of the z_i. Dunnett (1955) has evaluated this joint density for the case of $\rho_{ij} = \rho = .5$, by obtaining $F_n(z_1, z_2, \ldots, z_n; \{\rho_{ij}\})$ and integrating out s. Use of the Clark algorithm would provide a generalization of their result to the case of general $\{\rho_{ij}\}$, a natural application of which would be a generalization of Dunnett's test to the case of unequal sample sizes among the $k+1$ groups (*i.e.*, treatment groups and a single control).

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Table 1

Probability that n Standard Normal Random Variables with Common Correlation ρ, are Simultaneously $\leq h$.

A. Comparison with MULNOR

				MULNOR			Clark	
n	h	ρ	True[1]	Prob	Time[2]	Time[3]	Prob	Time[3]
3	2.0	.9	.96170	.96170	.196	.060	.96185	.0008
4	2.0	.5	.92845	.92845	7.275	1.760	.93088	.0012
4	2.0	.8	.94759	.94758	13.735	2.913	.94819	.0012
4	2.0	9	.95708	.95707	18.557	3.855	.95730	.0012
5[4]	1.0	.3	52111	.52113	40.461	8.900	.51341	.0016
7[4]	0.0	.9	.32967	.32965	NA	98040	.32921	.0026
7[4]	0.0	.2	.04043	.04038	NA	733	.04122	.0026

[1] Gupta (1963)

[2] Seconds on a DEC 2060

[3] Seconds on a COMPAQ 386-25, Weitek 3167, SVS FORTRAN

[4] Accuracy set to 10^{-3} instead of 10^{-4} for MULNOR

B. Higher Dimensional Integrals

				Clark	
n	h	ρ	True[1]	Prob	Time
10	0	.5	.09091	.08907	.0044
20	0	.5	.04762	.04657	.0134
40	0	.5	.02439	.02390	.0459

[1] $F_n(0, 0, \ldots, 0; \{.5\}) = \frac{1}{n+1}$

C. Tail Probabilities

n	h	ρ	True[1]	Clark
3	-2.5	.5	.00017	.00021
3	-2.5	.9	.00230	.00231
5	-2.5	.5	.00003	.00004
5	-2.5	.9	.00157	.00156
10	-2.5	.5	.00000	.00000
10	-2.5	.9	.00099	.00098

[1] Gupta (1963)

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