

AD-A229 129

**Approximating Multivariate Normal
Orthant Probabilities
ONR Technical Report**

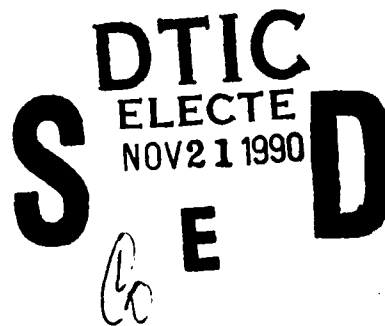
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May 1990

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Supported by the Cognitive Science Program, Office of Naval Research, under Grant #N00014-89-J-1104. Research in whole or in part is permitted for any purpose of the United States Government. Approved for public release; distribution unlimited.

REPORT DOCUMENTATION PAGE

Form Approved
OMB No 0704-0188

REPORT SECURITY CLASSIFICATION Unclassified		1b RESTRICTIVE MARKINGS	
SECURITY CLASSIFICATION AUTHORITY		3 DISTRIBUTION AVAILABILITY OF REPORT Approved for public release; distribution unlimited	
DECLASSIFICATION/DOWNGRADING SCHEDULE			
PERFORMING ORGANIZATION REPORT NUMBER(S) Biometric Lab Report #90-1		5 MONITORING ORGANIZATION REPORT NUMBER(S)	
NAME OF PERFORMING ORGANIZATION University of Illinois	6b OFFICE SYMBOL (if applicable)	7a NAME OF MONITORING ORGANIZATION Cognitive Science Research Program Office of Naval Research (Code 1142CS)	
ADDRESS (City, State, and ZIP Code) Illinois State Psychiatric Institute 529W 601 West Taylor Street Chicago, Illinois 60612		7b ADDRESS (City, State, and ZIP Code) 800 N. Quincy Street Arlington, Virginia 22217-5000	
NAME OF FUNDING/SPONSORING ORGANIZATION	8b OFFICE SYMBOL (if applicable)	9 PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER N 00014-89-J-1104	
ADDRESS (City, State, and ZIP Code)		10 SOURCE OF FUNDING NUMBERS	
		PROGRAM ELEMENT NO 61153N	PROJECT NO RR042046
		TASK NO RR04204-01	WORK UNIT ACCESSION NO 4421553

TITLE (Include Security Classification)

Approximating Multivariate Normal Orthant Probabilities

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TYPE OF REPORT Interim	13b TIME COVERED FROM 6/01/89 to 6/01/90	14 DATE OF REPORT (Year, Month, Day) June 1, 1990	15 PAGE COUNT
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SUPPLEMENTARY NOTATION

To be submitted for publication in Technometrics

16a SUBJECT TERMS (Continue on reverse if necessary and identify by block number)		
FIELD	GROUP	SUB GROUP
05	09	

ABSTRACT (Continue on reverse if necessary and identify by block number)

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

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

where $\{\rho_{ij}\}$ represents the $n \times n$ symmetric correlation matrix of the x_i 's, and $f(x_1, x_2, \dots, x_n; \{\rho_{ij}\})$ 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

DISTRIBUTION AVAILABILITY OF ABSTRACT ☒ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT ☐ DTIC USERS		21 ABSTRACT SECURITY CLASSIFICATION Unclassified	
NAME OF RESPONSIBLE INDIVIDUAL Dr. Charles Davis		22b TELEPHONE (Include Area Code) 202/696-4046	22c OFFICE SYMBOL ONR 1142PT

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

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 $n \leq 7$.

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NTIS GRA&I	☒
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Distribution/	
Availability Codes	
Dist	Avail and/or Special
A-1	



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

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

where $\{\rho_{ij}\}$ represents the $n \times n$ correlation matrix of the x_i 's, and $f(x_1, x_2, \dots, x_n; \{\rho_{ij}\})$ 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

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

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. (kP)

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

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

where $\{\rho_{ij}\}$ represents the $n \times n$ symmetric correlation matrix of the x_i 's, and $f(x_1, x_2, \dots, x_n; \{\rho_{ij}\})$ 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

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

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 Secrest, 1966). It should be noted that when $\rho_{ij} = \rho$ for all i, j , then

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

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

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

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^{-3} accuracy on a computer that 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 computationally tractable for $n > 10$.

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

$$F_n = Pr(x_1 \leq h_1, x_2 \leq h_2, \dots, x_n \leq h_n) \quad (5)$$

If $h_1 \dots h_n = h = 0$, 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

$$F_n^0 = Pr\{max(x_1, \dots, x_n) \leq 0\} \quad (6)$$

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

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

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 $max(x_1, \dots, x_n)$ 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 $max(x_1, \dots, x_n)$ 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 $F_n(x_1, x_2, \dots, x_n; \{\rho_{ij}\})$. We begin by reviewing Clark's original formulae.

2 The Clark Algorithm

Let any three successive components from an n -variate vector, 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:

$$\text{set} \quad z_{i+1} = (\mu_i - \mu_{i+1})/\zeta_{i+1},$$

$$\text{where} \quad \zeta_{i+1}^2 = \sigma_i^2 + \sigma_{i+1}^2 - 2\sigma_i \sigma_{i+1} \rho_{i,i+1}.$$

$$\begin{aligned} \text{Then } P(y_{i+1} > \tilde{y}_i) &= P(y_{i+1} - \tilde{y}_i > 0) \\ &= \Phi(-z_{i+1}) \end{aligned}$$

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,

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

variances

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

where

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

and correlation

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

Then,

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

is approximated by

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

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,

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

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,

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

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 $\max(y_1, \dots, y_4)$. 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 from .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 $\rho = .2, .3, .5$ 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 (Schervish, 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 $|\rho|$. 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 $t_i = z_i/s, (i = 1, 2, \dots, n)$ 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 $F_n(z_1, z_2, \dots, z_n; \{\rho_{ij}\})$ 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

n	h	ρ	True ¹	MULNOR			Clark	
				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	10.461	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

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

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

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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