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Algorithm AS 251: Multivariate Normal Probability Integrals with Product Correlation Structure

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```

      DETMUL = 0.0
      DO 410 K = 1, KSET
        DETMUL = DETMUL + (DET(K) - DETALL) * (NG(K) - 1) / TWO
410  CONTINUE
C
      Calculate RHO and W2
C
      M = NT - KSET
      R1 = 0.0
      R2 = 0.0
      DO 420 K = 1, KSET
        R1 = R1 + ONE / (NG(K) - 1)
        R2 = R2 + ONE / (NG(K) - 1) ** 2
420  CONTINUE
      RHO = ONE - (R1 - ONE / M) * (2 * (NP ** 2) + 3 * NP - 1) /
      * (F6 * (NP + 1) * (KSET - 1))
      W2 = NP * (NP + 1) * ((NP - 1) * (NP + 2) * (R2 - ONE / M ** 2) -
      * F6 * (KSET - 1) * (1 - RHO) ** 2) / (F48 * RHO ** 2)
C
      MDF = (KSET - 1) * MP
      CHI = -TWO * RHO * DETMUL
      RETURN
      END

```

## Algorithm AS 251

### Multivariate Normal Probability Integrals with Product Correlation Structure

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**Keywords:** Multinomial; Multivariate normal; Multivariate Student distribution; Product correlation structure

## Language

Fortran 77

### Description and Purpose

Let  $X_1, X_2, \dots, X_N$  be multinormal with zero means, unit variances and correlation structure defined by

$$\rho_{IJ} = b_I b_J \quad (I \neq J; -1 < b_I < 1). \quad (1)$$

The algorithm provides an approximation for

$$\text{PROB} = \Pr[(X_1, \dots, X_N) \in \mathbb{R}] \quad (2)$$

with specified error bound, where  $\mathbb{R}$  is a subset of  $N$ -dimensional space of the form

$$\mathbb{R} = \{(X_1, \dots, X_N): B(I) \leq X_I \leq A(I), \text{ for } I = 1, \dots, N\}, \quad (3)$$

where  $B(I) < A(I)$  are finite or infinite real numbers.

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If the mean  $\mu_i$  of the  $i$ th co-ordinate is not zero or its standard deviation  $\sigma_i$  is not unity, then  $\mu_i$  must be subtracted from  $A(I)$  and  $B(I)$  and the results divided by  $\sigma_i$  before using the algorithm. Thus, our set-up is identical with that considered by Schervish (1984) except for the special correlation structure that is assumed here. The advantage of the present algorithm over Schervish's, when the product correlation structure specified by equation (1) holds, is that computing times are reduced considerably. The computing times for Schervish's algorithm increase rapidly with  $N$ , making his algorithm impractical to use for dimensions much higher than 5 or 6. With the present algorithm, in contrast, no practical limitation is imposed by the value of  $N$ .

Although the use of the present algorithm is restricted to problems where the correlation structure (1) holds, this restriction is satisfied in many practical problems. For example, the case where all the correlation coefficients are equal to a common value  $\rho \geq 0$  occurs frequently and may be handled by defining  $b_i = \sqrt{\rho}$ . The correlation structure given by  $b_i = 1/\sqrt{1 + n_0/n_i}$  arises in multiple comparisons between  $N$  treatments and a control, where  $n_0$  and  $n_i$  are the sample sizes in the control and  $i$ th treatment groups (Dunnnett, 1955). The same correlation structure arises in the method of Hsu (1984) for obtaining simultaneous upper confidence limits on the differences between  $N + 1$  treatment means and the unknown best mean.

Suppose that  $V$  is distributed independently of  $X_1, X_2, \dots, X_N$  as a  $\chi^2$  random variable with  $v$  degrees of freedom and define  $T_i = (X_i + \delta_i)/\sqrt{(V/v)}$  for  $i = 1, \dots, N$  where the  $\delta_i$  are constants. Then  $T_1, T_2, \dots, T_N$  have a joint non-central multivariate Student distribution with correlation matrix  $\{\rho_{ij}\}$ , degrees of freedom  $v$  and non-centrality vector  $(\delta_1, \dots, \delta_N)$ . In certain applications, the value of

$$\text{PROB} = \Pr[B(I) \leq T_i \leq A(I); i = 1, \dots, N] \quad (4)$$

may be required instead of equation (2). This can be determined by expressing it as

$$\text{PROB} = \int_0^\infty G_N\{yB(I) - \delta_i, yA(I) - \delta_i; i = 1, \dots, N\} q_v(y) dy \quad (5)$$

where  $G_N\{B(I); A(I); i = 1, \dots, N\}$  denotes the corresponding multivariate normal probability and

$$q_v(y) = 2(v/2)^{v/2} y^{v-1} \exp(-vy^2/2)/\Gamma(v/2)$$

is the density function of  $\sqrt{(V/v)}$ . This integral can be evaluated using an appropriate numerical integration routine, such as the International Mathematical and Statistical Libraries' (1987a) QDAGI, employing either the present algorithm or that of Schervish to evaluate the function in the integrand depending on whether or not the product correlation structure holds. Anyone desiring a subroutine of 60 lines developed by the author for computing multivariate Student probability integrals given by equation (4) using QDAGI may obtain a listing of it from the author.

### Numerical Method

The random variables  $X_1, X_2, \dots, X_N$  can be expressed in terms of  $N + 1$  independent standard normal variates  $Y_1, \dots, Y_N, Z$  by setting  $X_i = \sqrt{(1 - b_i^2)} Y_i + b_i Z; i = 1, 2, \dots, N$ . This enables the probability (2) to be written as a single integral; see Dunnnett and Sobel (1955) or Curnow and Dunnnett (1962). The resulting integral may be written

$$\begin{aligned} \text{PROB} = & \frac{1}{\sqrt{\pi}} \int_0^\infty \left[ \prod_{i=1}^N \left\{ \Phi\left(\frac{A(I) - \sqrt{2} b_i z}{\sqrt{(1 - b_i^2)}}\right) - \Phi\left(\frac{B(I) - \sqrt{2} b_i z}{\sqrt{(1 - b_i^2)}}\right) \right\} \right. \\ & \left. + \prod_{i=1}^N \left\{ \Phi\left(\frac{A(I) + \sqrt{2} b_i z}{\sqrt{(1 - b_i^2)}}\right) - \Phi\left(\frac{B(I) + \sqrt{2} b_i z}{\sqrt{(1 - b_i^2)}}\right) \right\} \right] \exp(-z^2) dz, \end{aligned} \quad (6)$$

where  $\Phi(\cdot)$  is the cumulative distribution function (CDF) of the standardized univariate normal distribution. MVNPRD uses Simpson's rule to compute an approximation to equation (6), in such a way that a prescribed accuracy EPS is achieved.

To approximate the integral of a function  $f(z)$  over an interval  $[a, b]$  using Simpson's rule, the value of the function is computed at the two end points and at the midpoint of the interval. The approximate value of the integral is given by

$$\left\{ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right\} \frac{b-a}{6} \quad (7)$$

and a bound on its error is

$$f_4(a, b)(b-a)^5/2880, \quad (8)$$

where  $f_4(a, b)$  is a bound on the absolute value of the fourth derivative of  $f(z)$  over the interval: for example, see Shampine and Allen (1973).

MVNPRD computes these for the function in the integrand of equation (6) over intervals of initial width HINC, which are subdivided into smaller intervals if necessary so that the sum of their error bounds does not exceed a determined amount EL for each interval. The value of EL is chosen for each interval so that the sum of the error bounds over all the intervals of width HINC up to a maximum value  $z_u$  of  $z$ , added to a bound on the error arising from neglecting values  $z$  greater than  $z_u$ , is less than EPS.

The prescribed accuracy bound EPS is apportioned into an amount 0.1EPS to bound the error from neglecting the upper tail and the remaining amount 0.9EPS which is divided according to the number of intervals of width HINC that there are between zero and  $z_u$ . The number of these intervals determines the initial value for EL but, to decrease the amount of computing necessary, the value of EL is increased for each interval after the first by the amount of the excess of the value EL assigned to the previous interval over the error bound actually achieved.

Other values were tried for the constant 0.1 used to apportion EPS but there was little effect on the timing and accuracy of the computations over a range of values around the value chosen.

The values of the derivatives of the two product expressions in the integrand of equation (6) are denoted by FOU1 and GOU1 respectively in the program. Over each interval or subinterval, the bound on the absolute value of the fourth derivative of the function is approximated by fitting a quadratic function to the fourth derivative values at the midpoint and two end points and by taking the largest absolute value over the interval. This results in the computed bounds being approximate rather than mathematically guaranteed, but numerical computations indicate that the approximate bounds are usually very near to the correct bounds based on the actual maximum of the fourth derivative over the intervals (see the example displayed in Table 3, later).

The width HINC of the initial Simpson's rule intervals may be chosen by the user, or the value 0.0 entered which will invoke a default value. The default value chosen is 0.24 which was found to be a satisfactory compromise between a very small value which would entail a large number of computations and a large value for which the quadratic approximation for the maximum absolute value of the fourth derivative might be in question. If any of the values of  $b_i$  are near  $\pm 1$ , the user is advised to enter a smaller value for HINC than its default value.

There is an option to omit the computation of the fourth derivatives. The reason for this is that a large part of the total computing time is devoted to this and it can become excessive for values of  $N$  greater than 8–10. The user forgoes strict control over the error when this option is exercised. However, a bound is determined by computing for each interval or subinterval the value obtained by halving the width of the interval and applying Simpson's rule to each half: the absolute value of the difference between the result for the whole interval and the sum of the results for the two halves is used as an intuitive bound.

The case where some  $b_i = 0$ , which means that these variables have zero correlation with the other variables, is computed by factoring out the contributions of these variables to PROB and computing them as univariate normal integrals. Thus, MVNPRD uses numerical integration only for the variables that have non-zero values of  $b_i$ .

### Structure

The structure was chosen to be as close as possible to that used by Schervish (1984) for his algorithm MULNOR and is as follows.

*SUBROUTINE MVNPRD(A, B, BPD, EPS, N, INF, IERC, HINC, PROB, BOUND, IFAULT)*

#### *Formal parameters*

<i>A</i>	Real array ( $N$ )	input:	the upper limits of integration
<i>B</i>	Real array ( $N$ )	input:	the lower limits of integration
<i>BPD</i>	Real array ( $N$ )	input:	the values of $b_i$ defining the correlation structure
<i>EPS</i>	Real	input:	the desired accuracy
<i>N</i>	Integer	input:	the number of dimensions (the maximum value is 50; to increase it, change the values of NN in the two parameter statements in MVNPRD and PFUNC)
<i>INF</i>	Integer array ( $N$ )	input:	INF( $I$ ) = 0 if the $I$ th range of integration is $(B(I), \infty)$ ; INF( $I$ ) = 1 if the $I$ th range of integration is $(-\infty, A(I))$ ; INF( $I$ ) = 2 if the $I$ th range of integration is $(B(I), A(I))$
<i>IERC</i>	Integer	input:	method of error control: IERC = 1 if strict error control based on the fourth derivative is to be used; IERC = 0 if intuitive error control based on halving the intervals is to be used
<i>HINC</i>	Real	input:	interval width for Simpson's rule (enter

			HINC = 0.0 to invoke the default value 0.24)
<i>PROB</i>	Real	output:	the approximation to the $N$ -variate probability
<i>BOUND</i>	Real	output:	the bound on the actual error of the approximation: if IERC = 1, it is an actual bound based on the fourth derivative; if IERC = 0, it is an intuitive bound based on halving each interval or subinterval
<i>IFault</i>	Integer	output:	a fault indicator: = 1 if $N < 1$ or $N > 50$ ; = 2 if any $BPD(I) \geq 1$ or $BPD(I) \leq -1$ ; = 3 if any $INF(I) \neq 0, 1$ or $2$ ; = 4 if any $INF(I) = 2$ and $A(I) \leq B(I)$ ; = 5 if the number of terms computed exceeds the upper limit, set at 400 if IERC = 1 and 800 if IERC = 0; = 6 if a fault occurs in normal subroutines; = 7 if subintervals are too narrow or too many; = 8 if <i>BOUND</i> exceeds EPS; = 0 otherwise

### Auxiliary Algorithms

Function PFUNC calculates the value of the function in the integrand of equation (6) and the value of its fourth derivative, and is provided as part of the algorithm. Also provided is a subroutine ASSIGN which calculates the derivatives of the univariate normal CDFs shown in equation (6) and a function WMAX which determines the largest absolute value of a quadratic function fitted to three points. Additional functions needed, which must be provided by the user, are algorithms to compute the lower tail area of the standard normal distribution and to provide the value  $X$  such that the lower tail area of the standard normal is  $P$ . The functions ALNORM of Hill (1973) and PPND7 of Wichura (1988) are used here, but these may be replaced by S15ABF and G01CEF from the Numerical Algorithms Group's (1983) subroutine library or by ANORDF and ANORIN from the International Mathematical and Statistical Libraries' (1987b) subroutine library, if one of these libraries is available to the user.

### Accuracy and Timing

Table 1 shows comparative accuracies and timings of the two versions of MVNPRD, i.e. with and without strict error control, with those obtained using Schervish's MULNOR and with known or published values. A VAX 8600 computer system at McMaster University using single-precision arithmetic was used in the timing comparisons. The program has also been run on a CDC Cyber 170 computer at McMaster University and on a Prime 750 computer at University College of

TABLE 1  
Comparison of MVNPRD with MULNOR and with known or published results for cases of equal correlation  $\rho$  and identical ranges of integration

N	End points		$\rho$	EPS	Known or published result†	MVNPRD, with IERC = 0		MVNPRD, with IERC = 1		PROB	MULNOR BOUND	TIME‡
	B(1)	A(1)				PROB	BOUND	PROB	BOUND			
3	-5.0	5.0	0.5	$10^{-4}$	1.0	0.999952	0.000058	0.999952	0.000063	0.999974	0.000093	0.33
3	0.0	$\infty$	0.5	$10^{-4}$	0.25	0.250016	0.000047	0.250022	0.000048	0.249998	0.000082	0.02
3	0.0	$\infty$	$\frac{1}{3}$	$10^{-4}$	0.206130	0.206164	0.000060	0.206164	0.000065	0.206133	0.000086	0.02
3	-2.0	2.0	0.9	$10^{-4}$	Unknown	0.923402	0.000031	0.923402	0.000040	0.923401	0.000052	0.44
3	$-\infty$	2.0	0.9	$10^{-4}$	0.96170068	0.961701	0.000043	0.961719	0.000044	0.961696	0.000090	0.06
3	$-\infty$	2.0	0.5	$10^{-4}$	0.94253345	0.942493	0.000086	0.942492	0.000089	0.942526	0.000091	0.04
4	0.0	$\infty$	0.5	$10^{-4}$	0.2	0.200022	0.000059	0.200027	0.000061	0.199998	0.000080	0.83
4	$-\infty$	2.0	0.5	$10^{-4}$	0.92845060	0.928436	0.000040	0.928436	0.000044	0.928446	0.000090	2.37
6	$-\infty$	2.0	0.5	$10^{-5}$	0.90442100	0.904421	0.000005	0.904421	0.000005	§	§	§
9	$-\infty$	2.0	0.5	$10^{-5}$	0.87530598	0.875306	0.000003	0.875308	0.000005	§	§	§
14	$-\infty$	2.0	0.5	$10^{-5}$	0.83787227	0.837872	0.000005	0.837874	0.000005	§	§	§
24	$-\infty$	2.0	0.5	$10^{-5}$	0.78487259	0.784872	0.000003	§	§	§	§	§

†The result is known to be  $1/(N+1)$  for end points  $(0, \infty)$  and  $\rho = 0.5$ ; the result for  $N = 3$ ,  $\rho = \frac{1}{3}$  and end points  $(0, \infty)$  is given in Moran (1956); other numerical results shown are from tables by Milton (1963).

‡Times shown are in seconds of central processor unit time on a VAX 8600 computer using single-precision arithmetic.

§Not computed owing to the excessive computing time required.

Swansea, as well as on an IBM PC microcomputer using the Microsoft Fortran compiler.

All numerical results shown in Table 1 are for equal correlations and identical limits of integration for each variable. Slightly longer computing times are required by MVNPRD for unequal correlations or different limits of integration since then the product terms in the integrand of equation (6) will need to be recomputed for each value of  $I$ .

Table 2 shows the accuracy of MVNPRD for an unequal correlation case with limits of integration  $(0, \infty)$  for  $N = 3$ , where an exact expression is available (see Moran (1956)) for the probability integral, for a range of values for EPS.

Table 3 shows a particular example, giving the individual subintervals and the error bounds computed for each. The subintervals where the fourth derivative is not correctly given by the quadratic approximation fitted to the three values computed by

TABLE 2

*Values of PROB and BOUND obtained with MVNPRD for an unequal correlation case†*

EPS	MVNPRD, with IERC = 0			MVNPRD, with IERC = 1		
	PROB	BOUND	True error‡	PROB	BOUND	True error‡
$10^{-4}$	0.223 702 60	$0.48 \times 10^{-4}$	$0.42 \times 10^{-4}$	0.223 702 65	$0.54 \times 10^{-4}$	$0.42 \times 10^{-4}$
$10^{-5}$	0.223 668 88	$0.92 \times 10^{-5}$	$0.81 \times 10^{-5}$	0.223 661 48	$0.45 \times 10^{-5}$	$0.07 \times 10^{-5}$
$10^{-6}$	0.223 661 00	$0.67 \times 10^{-6}$	$0.19 \times 10^{-6}$	0.223 660 93	$0.75 \times 10^{-6}$	$0.12 \times 10^{-6}$
$10^{-7}$	0.223 660 84	$0.76 \times 10^{-7}$	$0.29 \times 10^{-7}$	0.223 660 81	$0.81 \times 10^{-7}$	$0.06 \times 10^{-7}$

†  $N = 3$ ,  $\rho_{12} = 0.5$ ,  $\rho_{13} = 0.4$ ,  $\rho_{23} = 0.3$  (or  $b_1 = \sqrt{6}/3$ ,  $b_2 = \sqrt{6}/4$ ,  $b_3 = \sqrt{6}/5$ ) and end points  $(0.0, \infty)$ .

‡ Exact result 0.223 660 81, computed from  $\frac{1}{2} - (\cos^{-1}\rho_{12} + \cos^{-1}\rho_{13} + \cos^{-1}\rho_{23})/4\pi$  (Moran, 1956).

TABLE 3

*Detailed results for a particular example ( $N = 3$ ,  $\rho = 0.9$ , end points  $(-2.0, 2.0)$  and  $EPS = 0.0001$ )*

Interval	Contribution to PROB	True error	Computed bound	Correct bound, if different†
0.00–0.24	0.265 703 51	0.000 003 45	0.000 003 74	—
0.24–0.48	0.237 049 92	0.000 001 57	0.000 002 73	—
0.48–0.72	0.188 608 69	–0.000 002 56	0.000 005 76	—
0.72–0.96	0.132 528 16	–0.000 005 00	0.000 007 24	0.000 006 90
0.96–1.08	0.004 612 31	0.000 000 54	0.000 000 80	—
1.08–1.20	0.029 890 98	0.000 000 72	0.000 000 83	0.000 000 82
1.20–1.32	0.016 346 61	–0.000 000 61	0.000 001 31	—
1.32–1.44	0.006 581 63	–0.000 001 37	0.000 001 41	0.000 001 45
1.44–1.56	0.001 761 66	–0.000 000 05	0.000 000 84	—
1.56–1.68	0.000 287 38	0.000 000 59	0.000 000 61	0.000 000 62
1.68–1.92	0.000 031 25	0.000 003 47	0.000 014 19	—
1.92– $\infty$	0.000 000 00	–0.000 000 03	0.000 000 27	—
	0.923 402 10	0.000 000 73	0.000 039 75	0.000 039 42

† Correct bound calculated from the actual maximum instead of the quadratic approximation to the maximum of the fourth derivative.



the algorithm are indicated, along with the correct values for the bounds based on the actual maximum of the fourth derivative.

### Acknowledgements

This algorithm had its origins in a program developed many years ago by the author when he was employed by Lederle Laboratories in Pearl River, USA. The author is greatly indebted to that organization for their support of his work.

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SUBROUTINE MVNPRD(A, B, BPD, EPS, N, INF, IERC, HINC, PROB, BOUND,
*              IFAULT)
C
C      ALGORITHM AS 251.1  APPL.STATIST. (1989), VOL.38, NO.3
C
C      FOR A MULTIVARIATE NORMAL VECTOR WITH CORRELATION STRUCTURE
C      DEFINED BY RHO(I,J) = BPD(I) * BPD(J), COMPUTES THE PROBABILITY
C      THAT THE VECTOR FALLS IN A RECTANGLE IN N-SPACE WITH ERROR
C      LESS THAN EPS.
C
C

```

```

INTEGER NN
PARAMETER (NN=50)
REAL A( * ), B( * ), BPD( * ), EPS, HINC, PROB, BOUND
INTEGER INF( * ), N, IERC, IFAULT
C
REAL ESTT(22), FV(5), FD(5), F1T(22), F2T(22), F3T(22), G1T(22),
*   G3T(22), PSUM(22), H(NN), HL(NN), BB(NN), ZERO, HALF, ONE,
*   TWO, FOUR, SIX, PT1, PT24, ONEP5, X2880, SMALL, DXMIN, SQRT2,
*   ERRRL, BI, START, Z, ADDN, EPS2, EPS1, ZU, Z2, Z3, Z4, Z5, ZZ,
*   ERFAC, EL, EL1, PART0, PART2, PART3, FUNC0, FUNC2, FUNCN, WT,
*   CONTRB, DLG, DX, DA, ESTL, ESTR, SUM, EXCESS, ERROR, PROBL,
*   SAFE
INTEGER INFT(NN), LDIR(22), I, NTM, NMAX, LVL, NR, NDIM
C
REAL ALNORM, PPND7
EXTERNAL ALNORM, PPND7
DATA ZERO, HALF, ONE, TWO, FOUR, SIX / 0.0, 0.5, 1.0, 2.0, 4.0,
*   6.0 /
DATA PT1, PT24, ONEP5, X2880 / 0.1, 0.24, 1.5, 2880.0 /
DATA SMALL, DXMIN, SQRT2 / 1.0E-10, 0.0000001, 1.41421356237310 /
C
CHECK FOR INPUT VALUES OUT OF RANGE.
C
PROB = ZERO
BOUND = ZERO
IFAULT = 1
IF (N .LT. 1 .OR. N .GT. NN) RETURN
DO 10 I = 1, N
  BI = ABS(BPD(I))
  IFAULT = 2
  IF (BI .GE. ONE) RETURN
  IFAULT = 3
  IF (INF(I) .LT. 0 .OR. INF(I) .GT. 2) RETURN
  IFAULT = 4
  IF (INF(I) .EQ. 2 .AND. A(I) .LE. B(I)) RETURN
10 CONTINUE
  IFAULT = 0
  PROB = ONE
C
CHECK WHETHER ANY BPD(I) = 0.
C
NDIM = 0
DO 20 I = 1, N
  IF (BPD(I) .NE. ZERO) THEN
    NDIM = NDIM + 1
    H(NDIM) = A(I)
    HL(NDIM) = B(I)
    BB(NDIM) = BPD(I)
    INFT(NDIM) = INF(I)
  ELSE
C
IF ANY BPD(I) = 0, THE CONTRIBUTION TO PROB FOR THAT
C VARIABLE IS COMPUTED FROM A UNIVARIATE NORMAL.
C
    IF (INF(I) .LT. 1) THEN
      PROB = PROB * (ONE - ALNORM(B(I), .FALSE.))
    ELSE IF (INF(I) .EQ. 1) THEN
      PROB = PROB * ALNORM(A(I), .FALSE.)
    ELSE
      PROB = PROB * (ALNORM(A(I), .FALSE.) -
        ALNORM(B(I), .FALSE.))
    END IF
    IF (PROB .LE. SMALL) PROB = ZERO
  END IF
20 CONTINUE
  IF (NDIM .EQ. 0 .OR. PROB .EQ. ZERO) RETURN
C
IF NOT ALL BPD(I) = 0, PROB IS COMPUTED BY SIMPSON'S RULE.

```

```

C      BUT FIRST, INITIALIZE THE VARIABLES.
C
      Z = ZERO
      IF (HINC .LE. ZERO) HINC = PT24
      ADDN = -ONE
      DO 30 I = 1, NDIM
        IF (INFT(I) .EQ. 2 .OR. (INFT(I) .NE. INFT(1) .AND.
*         BB(I) * BB(1) .GT. ZERO) .OR.
*         (INFT(I) .EQ. INFT(1) .AND. BB(I) * BB(1) .LT.
*         ZERO)) ADDN = ZERO
30 CONTINUE
C
C      THE VALUE OF ADDN IS TO BE ADDED TO THE PRODUCT EXPRESSIONS IN
C      THE INTEGRAND TO INSURE THAT THE LIMITING VALUE IS ZERO.
C
      PROB1 = ZERO
      NTM = 0
      NMAX = 400
      IF (IERC .EQ. 0) NMAX = NMAX * 2
      CALL PFUNC(Z, H, HL, BB, NDIM, INFT, ADDN, SAFE, FUNC0, NTM, IERC,
*      PART0)
      EPS2 = EPS * PT1 * HALF
C
C      SET UPPER BOUND ON Z AND APPORTION EPS.
C
      ZU = -PPND7(EPS2, IFAULT) / SQRT2
      IF (IFAULT .NE. 0) THEN
        IFAULT = 6
        RETURN
      END IF
      NR = IFIX(ZU / HINC) + 1
      ERFAC = ONE
      IF (IERC .NE. 0) ERFAC = X2880 / HINC ** 5
      EL = (EPS - EPS2) / FLOAT(NR) * ERFAC
      EL1 = EL
C
C      START COMPUTATIONS FOR THE INTERVAL (Z, Z + HINC).
C
40 ERROR = ZERO
      LVL = 0
      FV(1) = PART0
      FD(1) = SAFE
      START = Z
      DA = HINC
      Z3 = START + HALF * DA
      CALL PFUNC(Z3, H, HL, BB, NDIM, INFT, ADDN, FD(3), FUNCN, NTM,
*      IERC, FV(3))
      Z5 = START + DA
      CALL PFUNC(Z5, H, HL, BB, NDIM, INFT, ADDN, FD(5), FUNC2, NTM,
*      IERC, FV(5))
      PART2 = FV(5)
      SAFE = FD(5)
      WT = DA / SIX
      CONTRB = WT * (FV(1) + FOUR * FV(3) + FV(5))
      DLG = ZERO
      IF (IERC .NE. 0) THEN
        CALL WMAX(FD(1), FD(3), FD(5), DLG)
        IF (DLG .LE. EL) GO TO 90
        DX = DA
        GO TO 60
      END IF
      LVL = 1
      LDIR(LVL) = 2
      PSUM(LVL) = ZERO
C
C      BISECT INTERVAL. IF IERC = 1, COMPUTE ESTIMATE ON LEFT
C      HALF. IF IERC = 0, ON BOTH HALVES.
C

```

```

50 DX = HALF * DA
   WT = DX / SIX
   Z2 = START + HALF * DX
   CALL PFUNC(Z2, H, HL, BB, NDIM, INFT, ADDN, FD(2), FUNCN, NTM,
*       IERC, FV(2))
   ESTL = WT * (FV(1) + FOUR * FV(2) + FV(3))
   IF (IERC .EQ. 0) THEN
       Z4 = START + ONEP5 * DX
       CALL PFUNC(Z4, H, HL, BB, NDIM, INFT, ADDN, FD(4), FUNCN, NTM,
*       IERC, FV(4))
       ESTR = WT * (FV(3) + FOUR * FV(4) + FV(5))
       SUM = ESTL + ESTR
       DLG = ABS(CONTRB - SUM)
       EPS1 = EL / TWO ** (LVL - 1)
       ERR1 = DLG
   ELSE
       FV(3) = FV(2)
       FD(3) = FD(2)
       CALL WMAX(FD(1), FD(3), FD(5), DLG)
       ERR1 = DLG / TWO ** (5 * LVL)
       SUM = ESTL
       EPS1 = EL * (TWO ** LVL) ** 4
   END IF

C
C       STOP SUBDIVIDING INTERVAL WHEN ACCURACY IS SUFFICIENT,
C       OR IF INTERVAL TOO NARROW OR SUBDIVIDED TOO OFTEN.
C
   IF (DLG .LE. EPS1 .OR. DLG .LT. SMALL) GO TO 70
   IF (IFAUULT .EQ. 0 .AND. NTM .GE. NMAX) IFAULT = 5
   IF (ABS(DX) .LE. DXMIN .OR. LVL .GT. 21) IFAULT = 7
   IF (IFAUULT .NE. 0) GO TO 70

C
C       RAISE LEVEL. STORE INFORMATION FOR RIGHT HALF AND APPLY
C       SIMPSON'S RULE TO LEFT HALF.
C
60 LVL = LVL + 1
   LDIR(LVL) = 1
   F1T(LVL) = FV(3)
   F3T(LVL) = FV(5)
   DA = DX
   FV(5) = FV(3)
   IF (IERC .EQ. 0) THEN
       F2T(LVL) = FV(4)
       ESTT(LVL) = ESTR
       CONTRB = ESTL
       FV(3) = FV(2)
   ELSE
       G1T(LVL) = FD(3)
       G3T(LVL) = FD(5)
       FD(5) = FD(3)
   END IF
   GO TO 50

C
C       ACCEPT APPROXIMATE VALUE FOR INTERVAL.
C       RESTORE SAVED INFORMATION TO PROCESS
C       RIGHT HALF INTERVAL.
C
70 ERROR = ERROR + ERR1
80 IF (LDIR(LVL) .EQ. 1) THEN
   PSUM(LVL) = SUM
   LDIR(LVL) = 2
   IF (IERC .EQ. 0) DX = DX * TWO
   START = START + DX
   DA = HINC / TWO ** (LVL - 1)
   FV(1) = F1T(LVL)
   IF (IERC .EQ. 0) THEN
       FV(3) = F2T(LVL)
       CONTRB = ESTT(LVL)
   ELSE

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```

      FV(3) = F3T(LVL)
      FD(1) = G1T(LVL)
      FD(5) = G3T(LVL)
    END IF
    FV(5) = F3T(LVL)
    GO TO 50
  END IF
  SUM = SUM + PSUM(LVL)
  LVL = LVL - 1
  IF (LVL .GT. 0) GO TO 80
  CONTRB = SUM
  LVL = 1
  DLG = ERROR
90  PROB1 = PROB1 + CONTRB
  BOUND = BOUND + DLG
  EXCESS = EL - DLG
  EL = EL1
  IF (EXCESS .GT. ZERO) EL = EL1 + EXCESS
  IF ((FUNC0 .GT. ZERO .AND. FUNC2 .LE. FUNC0) .OR.
  * (FUNC0 .LT. ZERO .AND. FUNC2 .GE. FUNC0)) THEN
    ZZ = -SQRT2 * Z5
    PART3 = ABS(FUNC2) * ALNORM(ZZ, .FALSE.) + BOUND / ERFAC
    IF (PART3 .LE. EPS .OR. NTM .GE. NMAX .OR.
  *    Z5 .GE. ZU) GO TO 100
  END IF
  Z = Z5
  PART0 = PART2
  FUNC0 = FUNC2
  GO TO 40
100  PROB = (PROB1 - ADDN * HALF) * PROB
  BOUND = PART3
  IF (NTM .GE. NMAX .AND. IFAULT .EQ. 0) IFAULT = 5
  IF (BOUND .GT. EPS .AND. IFAULT .EQ. 0) IFAULT = 8
  RETURN
END
SUBROUTINE PFUNC(Z, A, B, BPD, N, INF, ADDN, DERIV, FUNCN, NTM,
  * IERC, RESULT)
C
C   ALGORITHM AS 251.2 APPL.STATIST. (1989), VOL.38, NO.3
C
C   COMPUTE FUNCTION IN INTEGRAND AND ITS 4TH DERIVATIVE.
C
  INTEGER NN
  PARAMETER (NN=50)
  REAL A( * ), B( * ), BPD( * ), Z, ADDN, DERIV, FUNCN, RESULT
  INTEGER INF( * ), N, NTM, IERC
C
  REAL FOU(NN), FOU1(4, NN), TMP(4), GOU(NN), GOU1(4, NN), FF(4),
  * GF(4), TERM(4), GERM(4), ZERO, ONE, TWO, THREE, FOUR, SIX,
  * EIGHT, TWELVE, SIXTN, SMALL, U, U1, U2, BI, HI, HLI, BP,
  * RSLT1, RSLT2, DEN, SQRT2, SQRTPI, PHI, PHI1, PHI2, PHI3, PHI4,
  * FRM, GRM
  INTEGER INFI, I, J, K, M, L, IK
C
  REAL ALNORM
  EXTERNAL ALNORM
  DATA ZERO, ONE, TWO, THREE, FOUR, SIX, EIGHT, TWELVE, SIXTN,
  * SMALL / 0.0, 1.0, 2.0, 3.0, 4.0, 6.0, 8.0, 12.0, 16.0,
  * 0.1E-12 /
  DATA SQRT2, SQRTPI / 1.41421356237310, 1.77245385090552 /
C
  DERIV = ZERO
  NTM = NTM + 1
  RSLT1 = ONE
  RSLT2 = ONE
  BI = ONE
  HI = A(1) + ONE
  HLI = B(1) + ONE

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      INFI = -1
      DO 60 I = 1, N
      IF (BPD(I) .EQ. BI .AND. A(I) .EQ. HI .AND. B(I) .EQ. HLI .AND.
*      INF(I) .EQ. INFI) THEN
        FOU(I) = FOU(I - 1)
        GOU(I) = GOU(I - 1)
        DO 10 IK = 1, 4
          FOUL(IK, I) = FOUL(IK, I - 1)
          GOUL(IK, I) = GOUL(IK, I - 1)
10      CONTINUE
      ELSE
        BI = BPD(I)
        HI = A(I)
        HLI = B(I)
        INFI = INF(I)
        IF (BI .EQ. ZERO) THEN
          IF (INFI .LT. 1) THEN
            FOU(I) = ONE - ALNORM(HLI, .FALSE.)
          ELSE IF (INFI .EQ. 1) THEN
            FOU(I) = ALNORM(HI, .FALSE.)
          ELSE
            FOU(I) = ALNORM(HI, .FALSE.) - ALNORM(HLI, .FALSE.)
          END IF
          GOU(I) = FOU(I)
          DO 20 IK = 1, 4
            FOUL(IK, I) = ZERO
            GOUL(IK, I) = ZERO
20      CONTINUE
      ELSE
        DEN = SQRT(ONE - BI * BI)
        BP = BI * SQRT2 / DEN
        IF (INFI .LT. 1) THEN
          U = -HLI / DEN + Z * BP
          FOU(I) = ALNORM(U, .FALSE.)
          CALL ASSIGN(U, BP, FOUL(1, I))
          BP = -BP
          U = -HLI / DEN + Z * BP
          GOU(I) = ALNORM(U, .FALSE.)
          CALL ASSIGN(U, BP, GOUL(1, I))
        ELSE IF (INFI .EQ. 1) THEN
          U = HI / DEN + Z * BP
          GOU(I) = ALNORM(U, .FALSE.)
          CALL ASSIGN(U, BP, GOUL(1, I))
          BP = -BP
          U = HI / DEN + Z * BP
          FOU(I) = ALNORM(U, .FALSE.)
          CALL ASSIGN(U, BP, FOUL(1, I))
        ELSE
          U2 = -HLI / DEN + Z * BP
          CALL ASSIGN(U2, BP, FOUL(1, I))
          BP = -BP
          U1 = HI / DEN + Z * BP
          CALL ASSIGN(U1, BP, TMP(1))
          FOU(I) = ALNORM(U1, .FALSE.) + ALNORM(U2, .FALSE.) -
*          ONE
          DO 30 IK = 1, 4
            FOUL(IK, I) = FOUL(IK, I) + TMP(IK)
30      CONTINUE
          IF (-HLI .EQ. HI) THEN
            GOU(I) = FOU(I)
            DO 40 IK = 1, 4
              GOUL(IK, I) = FOUL(IK, I)
40      CONTINUE
          ELSE
            U2 = -HLI / DEN + Z * BP
            CALL ASSIGN(U2, BP, GOUL(1, I))
            BP = -BP
            U1 = HI / DEN + Z * BP

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      GOU(I) = ALNORM(U1, .FALSE.) +
*          ALNORM(U2, .FALSE.) - ONE
      CALL ASSIGN(U1, BP, TMP(1))
      DO 50 IK = 1, 4
          GOU1(IK, I) = GOU1(IK, I) + TMP(IK)
50      CONTINUE
      END IF
      END IF
      END IF
      END IF
      RSLT1 = RSLT1 * FOU(I)
      RSLT2 = RSLT2 * GOU(I)
      IF (RSLT1 .LE. SMALL) RSLT1 = ZERO
      IF (RSLT2 .LE. SMALL) RSLT2 = ZERO
60 CONTINUE
      FUNCN = RSLT1 + RSLT2 + ADDN
      RESULT = FUNCN * EXP(-Z * Z) / SQRTPI
C
C      IF 4TH DERIVATIVE IS NOT WANTED, STOP HERE.
C      OTHERWISE, PROCEED TO COMPUTE 4TH DERIVATIVE.
C
      IF (IERC .EQ. 0) RETURN
      DO 70 IK = 1, 4
          FF(IK) = ZERO
          GF(IK) = ZERO
70 CONTINUE
      DO 100 I = 1, N
          FRM = ONE
          GRM = ONE
          DO 80 J = 1, N
              IF (J .EQ. 1) GO TO 80
              FRM = FRM * FOU(J)
              GRM = GRM * GOU(J)
              IF (FRM .LE. SMALL) FRM = ZERO
              IF (GRM .LE. SMALL) GRM = ZERO
80          CONTINUE
          DO 90 IK = 1, 4
              FF(IK) = FF(IK) + FRM * FOU1(IK, I)
              GF(IK) = GF(IK) + GRM * GOU1(IK, I)
90          CONTINUE
100 CONTINUE
      IF (N .LE. 2) GO TO 230
      DO 130 I = 1, N
          DO 120 J = I + 1, N
              TERM(2) = FOU1(1, I) * FOU1(1, J)
              GERM(2) = GOU1(1, I) * GOU1(1, J)
              TERM(3) = FOU1(2, I) * FOU1(1, J)
              GERM(3) = GOU1(2, I) * GOU1(1, J)
              TERM(4) = FOU1(3, I) * FOU1(1, J)
              GERM(4) = GOU1(3, I) * GOU1(1, J)
              TERM(1) = FOU1(2, I) * FOU1(2, J)
              GERM(1) = GOU1(2, I) * GOU1(2, J)
              DO 110 K = 1, N
                  IF (K .EQ. I .OR. K .EQ. J) GO TO 110
                  CALL TOOSML(1, TERM, FOU(K))
                  CALL TOOSML(1, GERM, GOU(K))
110          CONTINUE
              FF(2) = FF(2) + TWO * TERM(2)
              FF(3) = FF(3) + TWO * TERM(3) * THREE
              FF(4) = FF(4) + TWO * (TERM(4) * FOUR + TERM(1) * THREE)
              GF(2) = GF(2) + TWO * GERM(2)
              GF(3) = GF(3) + TWO * GERM(3) * THREE
              GF(4) = GF(4) + TWO * (GERM(4) * FOUR + GERM(1) * THREE)
120          CONTINUE
130 CONTINUE
      DO 170 I = 1, N
          DO 160 J = I + 1, N
              DO 150 K = J + 1, N

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      TERM(3) = FOUL(1, I) * FOUL(1, J) * FOUL(1, K)
      TERM(4) = FOUL(2, I) * FOUL(1, J) * FOUL(1, K)
      GERM(3) = GOUL(1, I) * GOUL(1, J) * GOUL(1, K)
      GERM(4) = GOUL(2, I) * GOUL(1, J) * GOUL(1, K)
      IF (N .GT. 3) THEN
        DO 140 M = 1, N
          IF (M .EQ. I .OR. M .EQ. J .OR.
            *      M .EQ. K) GO TO 140
          CALL TOOSML(3, TERM, FOU(M))
          CALL TOOSML(3, GERM, GOU(M))
140      CONTINUE
        END IF
        FF(3) = FF(3) + SIX * TERM(3)
        FF(4) = FF(4) + SIX * TERM(4) * SIX
        GF(3) = GF(3) + SIX * GERM(3)
        GF(4) = GF(4) + SIX * GERM(4) * SIX
150      CONTINUE
160      CONTINUE
170      CONTINUE
      IF (N .LE. 3) GO TO 230
      DO 220 I = 1, N
        DO 210 J = I + 1, N
          DO 200 K = J + 1, N
            DO 190 M = K + 1, N
              TERM(4) = FOUL(1, I) * FOUL(1, J) * FOUL(1, K) *
                *      FOUL(1, M)
              GERM(4) = GOUL(1, I) * GOUL(1, J) * GOUL(1, K) *
                *      GOUL(1, M)
              IF (N .GT. 4) THEN
                DO 180 L = 1, N
                  IF (L .EQ. I .OR. L .EQ. J .OR. L .EQ. K .OR.
                    *      L .EQ. M) GO TO 180
                  CALL TOOSML(4, TERM, FOU(L))
                  CALL TOOSML(4, GERM, GOU(L))
180      CONTINUE
                END IF
                FF(4) = FF(4) + FOUR * SIX * TERM(4)
                GF(4) = GF(4) + FOUR * SIX * GERM(4)
190      CONTINUE
200      CONTINUE
210      CONTINUE
220      CONTINUE
C
230      CONTINUE
      PHI = EXP(-Z * Z) / SQRTPI
      PHI1 = -TWO * Z * PHI
      PHI2 = (FOUR * Z ** 2 - TWO) * PHI
      PHI3 = (-EIGHT * Z ** 3 + TWELVE * Z) * PHI
      PHI4 = (SIXTN * Z ** 2 * (Z ** 2 - THREE) + TWELVE) * PHI
      DERIV = PHI * (FF(4) + GF(4)) + FOUR * PHI1 * (FF(3) + GF(3)) +
        *      SIX * PHI2 * (FF(2) + GF(2)) +
        *      FOUR * PHI3 * (FF(1) + GF(1)) + PHI4 * FUNCN
      RETURN
      END
      SUBROUTINE ASSIGN(U, BP, FF)
C
C      ALGORITHM AS 251.3 APPL.STATIST. (1989), VOL.38, NO.3
C
C      COMPUTE DERIVATIVES OF NORMAL CDF'S.
C
      REAL FF(4), U, BP
      REAL U2, HALF, ONE, THREE, SQ2PI, T1, T2, T3, ZERO, UMAX, SMALL
      INTEGER I
C
      DATA HALF, ONE, THREE, SQ2PI / 0.5, 1.0, 3.0, 2.50662827463100 /
      DATA ZERO, UMAX, SMALL / 0.0, 8.0, 0.1E-07 /
      IF (ABS(U) .GT. UMAX) THEN
        DO 10 I = 1, 4

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      FF(I) = ZERO
10  CONTINUE
      ELSE
        U2 = U * U
        T1 = BP * EXP(-HALF * U2) / SQ2PI
        T2 = BP * T1
        T3 = BP * T2
        FF(1) = T1
        FF(2) = -U * T2
        FF(3) = (U2 - ONE) * T3
        FF(4) = (THREE - U2) * U * BP * T3
        DO 20 I = 1, 4
          IF (ABS(FF(I)) .LT. SMALL) FF(I) = ZERO
20  CONTINUE
      END IF
      RETURN
      END
      SUBROUTINE WMAX(W1, W2, W3, DLG)
C
C      ALGORITHM AS 251.4 APPL.STATIST. (1989), VOL.38, NO.3
C
C      LARGEST ABSOLUTE VALUE OF QUADRATIC FUNCTION FITTED
C      TO THREE POINTS.
C
      REAL W1, W2, W3, DLG
      REAL QUAD, QLIM, QMIN, ONE, TWO, B2C
      DATA ONE, TWO, QMIN / 1.0, 2.0, 0.00001 /
C
      DLG = MAX(ABS(W1), ABS(W3))
      QUAD = W1 - W2 * TWO + W3
      QLIM = MAX(ABS(W1 - W3) / TWO, QMIN)
      IF (ABS(QUAD) .LE. QLIM) RETURN
      B2C = (W1 - W3) / QUAD / TWO
      IF (ABS(B2C) .GE. ONE) RETURN
      DLG = MAX(DLG, ABS(W2 - B2C * QUAD * B2C / TWO))
      RETURN
      END
      SUBROUTINE TOOSML(N, FF, F)
C
C      ALGORITHM AS 251.5 APPL.STATIST. (1989), VOL.38, NO.3
C
C      MULTIPLY FF(I) BY F FOR I = N TO 4. SET TO ZERO IF TOO SMALL.
C
      REAL FF(4), F
      INTEGER N
      REAL ZERO, SMALL
      INTEGER I
      DATA ZERO, SMALL / 0.0, 0.1E-12 /
C
      DO 10 I = N, 4
        FF(I) = FF(I) * F
        IF (ABS(FF(I)) .LE. SMALL) FF(I) = ZERO
10  CONTINUE
      RETURN
      END

```