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Algorithm AS 106: The Distribution of Non-Negative Quadratic Forms in Normal Variables

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Source: Journal of the Royal Statistical Society. Series C (Applied Statistics), Vol. 26, No. 1

(1977), pp. 92-98

Published by: Wiley for the Royal Statistical Society Stable URL: http://www.jstor.org/stable/2346884

Accessed: 11-03-2015 18:12 UTC

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```
8 IF (J .EQ. NVAR) GOTO 10
      DO \ O \ K = 12, \ J1
      DO O L = J2, NVAR
      MAT(K, L) = MAT(K, L) +
     * MIJ * (MAT(I, K) * MAT(J, L) + MAT(K, J) * MAT(I, L))
    O CONTINUE
С
         POSITIONS WITH K AND L GREATER THAN J
   10 IF (J .EQ. NVAR) GOTO 12
      DO 11 K = J2, NVAR
      SAVE1 = MAT(I, K)
      SAVE2 = MAT(J, K)
      MAT(I, K) = SAVE1 - MJJ * SAVE2

MAT(J, K) = SAVE2 - MII * SAVE1
      MAT(K, K) = MAT(K, K) +
     * MIJ * (MAT(I, K) * SAVE2 + MAT(J, K) * SAVE1)
      IF (K .EQ. NVAR) GOTO 12
      K1 = K + 1
      DO 11 L = K1, NVAR
      MAT(K, L) = MAT(K, L) +
     * MIJ * (MAT(I, K) * MAT(J, L) + MAT(J, K) * MAT(I, L))
   11 CONTINUE
   12 RETURN
   13 IFAULT = 1
      RETURN
      END
```

Algorithm AS 106

The Distribution of Non-negative Quadratic Forms in Normal Variables

By J. SHEIL† and I. O'MUIRCHEARTAIGH

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Keywords: QUADRATIC FORM; DISTRIBUTION; NON-NEGATIVE DEFINITE

LANGUAGE

ISO Fortran

DESCRIPTION AND PURPOSE

Given that the *n*-dimensional vector z has a multivariate normal distribution with expected value vector μ and non-singular covariance matrix V, this algorithm computes the distribution function of the quadratic form $(z+a)^T C(z+a)$ for a fixed vector a and symmetric positive definite, or positive semi-definite, matrix C. The value of the density is also presented in the output. The quadratic form is expressed as an infinite series in central χ^2 distribution functions: both the distribution functions and the series coefficients are evaluated recursively.

THEORY AND NUMERICAL METHOD $n = \text{dimensionality of } \mathbf{z}$.

By making the linear transformations

$$z-\mu = L^T Rx$$
, $a+\mu = L^T Rb$,

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it has been shown by Ruben (1962) that

$$P\{(\mathbf{z}+\mathbf{a})^{\mathrm{T}} \mathbf{C}(\mathbf{z}+\mathbf{a}) \leq t\} = P\{(\mathbf{x}+\mathbf{b})^{\mathrm{T}} \mathbf{A}(\mathbf{x}+\mathbf{b}) \leq t\},$$

where the components of the vector \mathbf{x} are uncorrelated standard normal variables and where \mathbf{L} is the upper triangular matrix defined by $\mathbf{V} = \mathbf{L}^T \mathbf{L}$, \mathbf{R} is the matrix whose columns are the eigenvectors of \mathbf{LCL}^T , and $\mathbf{A} = \deg(\alpha_i)$ is a diagonal matrix whose elements α_i are the eigenvalues of \mathbf{LCL}^T .

If f(n', y) denotes the probability density of a central χ^2 with n' degrees of freedom and F(n', y) the corresponding distribution function, then combining results from Ruben (1962) and Kotz et al. (1967)

$$\begin{split} P\{(\mathbf{z}+\mathbf{a})^{\mathrm{T}} \, \mathbf{C}(\mathbf{z}+\mathbf{a}) \leqslant t\} &= \sum_{k=0}^{\infty} c_k \, F(n'+2k,t/\beta), \quad t > 0, \\ &= 0, \qquad \qquad t \leqslant 0, \end{split}$$

where β is a distribution free constant, and n' is the rank of C. If $0 < \beta < 2 \min_i(\alpha_i)$, the above series is uniformly absolutely convergent for all t > 0, where i = 1, 2, ..., n'.

This algorithm uses $\beta = 0.90625 \alpha_{\min}$ which makes the above series a mixture representation (Robbins and Pitman, 1949). Therefore,

$$c_k \geqslant 0$$
, $\sum_{k=0}^{\infty} c_k = 1$.

If the series is truncated after N terms, then by the monotonic decreasing property of the χ^2 functions

$$\sum_{k=N+1}^{\infty} c_k F(n'+2k,y/\beta) < \left(1 - \sum_{k=0}^{N} c_k\right) F(n'+2N,y/\beta).$$

The series coefficients are evaluated as follows:

$$c_0 = A e^{-\lambda/2}$$
 $c_k = k^{-1} \sum_{r=0}^{k-1} g_{k-r} c_r$

where

$$A = \prod_{j=1}^{n'} \sqrt{(\beta/\alpha_j)}, \quad \lambda = \sum_{j=1}^{n'} b_j^2, \quad g_m = \frac{m}{2} \sum_{j=1}^{n'} b_j^2 \gamma_j^{m-1} + \frac{1}{2} \sum_{j=1}^{n'} (1 - mb_j^2) \gamma_j^m \quad (m \ge 1)$$

and $\gamma_j = 1 - \beta/\alpha_j$ (j = 1, 2, ..., n'). The χ^2 distribution functions are computed recursively using the relationships

$$F(\nu, a) = F(\nu - 2, a) - 2f(\nu, a) \quad (\nu \ge 3),$$

$$f(\nu, a) = \frac{\mathbf{a}}{(\nu - 2)} f(\nu - 2, a) \quad (\nu \ge 3),$$

$$F(2, a) = 1 - e^{-a/2}, \quad f(2, a) = \frac{1}{2} e^{-a/2},$$

$$F(1, a) = 2\Phi(\sqrt{a}) - 1, \quad f(1, a) = e^{-a/2}/\sqrt{(2\pi a)},$$

where $\Phi(.)$ is the standard normal distribution function and is evaluated using Algorithm AS 66 (Hill, 1973).

The method of Cholesky (Ralston, 1965) is used in the triangular decomposition of the matrix V.

STRUCTURE

SUBROUTINE QDIST (N, ETA, PRECIS, V, C, XA, EXPT, XLIM, XL, A, VALU, GAMA, B, ANS, DNSTY, NN, IFAULT)

| Formal parameters | | | |
|---------------------------|---------------------|-------------|--|
| N | Integer | input: | dimensionality |
| ETA | Real | input: | set ETA = smallest positive number represent- |
| | | | able in the machine |
| PRECIS | Real | input: | <i>PRECIS</i> = smallest positive number for which |
| | | | $1 + PRECIS \neq 1$ |
| V | Real array (N, N) | input: | covariance matrix |
| \boldsymbol{C} | Real array (N, N) | input: | symmetric matrix of the quadratic form |
| XA | Real array (N) | input: | fixed vector of quadratic form |
| EXPT | Real array (N) | input: | expected value vector |
| XLIM | Real | input: | value of t for which probability is required |
| XL | Real array (N, N) | work space: | work matrix holding the upper triangular |
| | | | matrix L |
| \boldsymbol{A} | Real array (N, N) | work space: | work matrix. Contains LCL ^T in call to AS 60. |
| | | | Holds eigenvectors of LCL ^T as output from |
| | | | AS 60 |
| VALU | Real array (N) | work space: | work vector holding eigenvalues of LCL ^T |
| GAMA | Real array (N) | work space: | work vector |
| $\boldsymbol{\mathit{B}}$ | Real array (N) | work space: | holds elements of non-centrality vector |
| ANS | Real | output: | resultant probability |
| DNSTY | Real | output: | density ordinate at t |
| NN | Integer | output: | numbers of terms used in series |
| IFAULT | Integer | output: | fault indicator |
| | | | IFAULT = 0: no error |

IFAULI = 0: no error

IFAULT = 1: XLIM not positive IFAULT = 2: V is not positive definite

IFAULT = 3: more than MITS iterations are required in LRVT. MITS is set to

30 in a DATA statement, but may

be reset by the user

IFAULT = 4: C is not positive semi-definite

IFAULT = 5: More than 100 terms required in the series expansion. The dimensions of COEFA and COEFB can be increased by the user if

required

AUXILIARY ALGORITHMS

Algorithm AS 60 (Sparks and Todd, 1973a) is used to find eigenvalues and corresponding eigenvectors and the standard normal integral is evaluated by using Algorithm AS 66 (Hill, 1973).

ACCURACY

The series is terminated when the maximum possible contribution from the remaining terms is less than 10^{-5} . If greater accuracy is required the assignment to *TEST* 2 in the *DATA* statement should be decreased.

In view of the comments on accuracy in Sparks and Todd (1973b) all tests were carried out using double precision arithmetic.

The algorithm was tested on a UNIVAC 1106 computer and the results compared with those published in Grad and Solomon (1955). A detailed description of results is in O'Muircheartaigh and Sheil's forthcoming paper.

ADDITIONAL COMMENT

When V and C are both unit matrices or when $V = C^{-1}$ this algorithm may be used to find the distribution function of both central and non-central χ^2 random variables.

PRECISION

The version of the algorithm given below is in single precision. To obtain a double precision version it is necessary to make the following alteration to *QDIST*.

- 1. Change REAL to DOUBLE PRECISION.
- 2. Change the real constant assignments in the *DATA* statements to double precision values.
- 3. Replace SQRT by DSQRT in the statement before the DO 50 loop, before the label 50, in the DO 150 loop and in the statement following label 180.
- 4. Change EXP to DEXP in the statement immediately following the label 150, in the second statement following label 180 and at label 200.
- 5. Replace ALOG by DLOG in the second statement after the label 180.

The value assigned to the local variable CONST is $\ln \sqrt{(2\pi)}$. When a double precision version of QDIST is being employed, the user may add some more digits (provided the compiler allows it).

To obtain double precision versions of *LRVT*, *TDIAG* and *ALNORM* see Hill (1973) and Sparks and Todd (1973a).

ACKNOWLEDGEMENTS

The authors wish to thank Dr I. D. Hill and the referee for their helpful comments on an earlier version of the algorithm.

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```
SUBROUTINE QDIST(N, ETA, PRECIS, V, C, XA, EXPT, XLIM, XL, A,

* VALI, GAMA, B, ANS, DNSTY, PN, IFAULT)

C

ALGORITHM AS 106 APPL. STATIST. (1977), VOL.26, NO.1

C

FINDS THE DISTRIBUTION OF NON-NEGATIVE DEFINITE QUADRATIC FORMS
IN NORMAL VARIABLES

C

REAL

V(N, N), C(N, N), A(N, N), XL(N, N), EXPT(N), XA(N), VALU(N),
GAMA(N), B(N), ETA, PRECIS, XLIM, ANS, DNSTY, TOL, BETA, AP,
XLMDA, XMU, AO, XTOP, PANS, DANS, DN, XN, XNN, BJ2NN, TERM,
ZERO, CNE, TWO, MULT, TEST2, CONST, SUM, XN1, TOTAI, ALNORM,
COEFA(100), COEFB(100)
```

```
DATA ZERO /0.0/, ONE /1.0/, TWO /2.0/, MULT /0.90625/
      DATA TEST2 /1.0E-5/, CONST /0.9189385332/
      IFAULT = 1
      IF (XLIM .LE. ZERO) RETURN
С
         TRIANGULAR FACTORISATION OF COVAR. MATRIX - V = ML - L
С
         UPPER TRIANGULAR M IS TRANSPOSE OF L
С
      XL(1, 1) = SQRT(V(1, 1))
      DO 50 J = 2, N
      JJ = J - 1
      DO 25 I = 1, JJ
      XL(I, J) = V(I, J) / XL(I, I)
      IF (I .LE. 1) GOTO 25
      KK = I - 1
      DO 20 K = 1, KK
   20 XL(I, J) = XL(I, J) - XL(K, I) * XL(K, J) / XL(I, I)
   25 CONTINUE
      XL(J, J) = V(J, J)
      DO 30 K = 1, JJ
   30 XL(J, J) = XL(J, J) - XL(K, J) ** 2
      IFAULT = 2
      IF (XL(J, J) .LE. ZERO) RETURN
      XL(J, J) = SQRT(XL(J, J))
   50 CONTINUE
С
         COMPUTE THE SYMMETRIC MATRIX A = LCM
С
      DO 85 J = 1, N
      DO 85 I = 1, J
      A(I, J) = ZERO
      DO 80 K = I, N
      DO SO L = J, N
   80 A(I, J) = A(I, J) + XL(I, K) * C(K, L) * XL(J, L)
      A(J, I) = A(I, J)
   85 CONTINUE
С
         STORE EIGENVALUES OF LCM, IN ORDER OF DESCENDING
С
         MAGNITUDE, IN ARRAY-VALU. PUT CORRESPONDING
С
         EIGENVECTORS INTO THE ARRAY-A
С
      TOL = ETA / PRECIS
      CALL TDIAG(N, TOL, A, B, GAMA, A)
      CALL LRVT(N, PRECIS, B, GAMA, A, IER)
      IFAULT = 3
      IF (IER .EQ. 1) RETURN
      IFAULT = 4
      N1I = N + 1
      DO \ OO \ I = 1, N
      N1I = N1I - 1
      VALU(I) = B(N1I)
      IF (VALU(I) .LT. ZERO) RETURN
   90 CONTINUE
С
С
         INVERT THE UPPER TRIANGULAR MATRIX - L
      DO 100 I = 1, N
  100 XL(I, I) = ONE / XL(I, I)
      JEND = N + 1
      DO 120 J = 2, N
      JEND = JEND - 1
      IEND = JEND
      ITOP = JEND - 1
      DO 120 I = 1, ITOP
      KBOT = IEND
      IEND = IEND - 1
      SUM = ZERO
      DO 110 K = KBOT, JEND
  110 SUM = SUM + XL(IEND, K) * XL(K, JEND)
      XL(IEND, JEND) = -SUM * XL(IEND, IEND)
  120 CONTINUE
```

```
С
          COMPUTE THE NON-CENTRALITY VECTOR - B
       N1I = N + 1
       DO 130 I = 1, N
       N1I = N1I - 1
       B(I) = ZERO
       DO 130 K = 1, N
       DO 130 J = 1, K
       B(I) = B(I) + A(K, N1I) * XL(J, K) * (XA(J) + EXPT(J))
   130 CONTINUE
 С
С
          NOW COMPUTE THE PROGRAM PARAMETERS USED TO DETERMINE
С
          COEFFS IN SERIES
C
       DO 135 I = 1, N
       IF (VALU(I) .EQ. ZERO) GOTO 140
   135 CONTINUE
       NPRIME = N
       GOTO 145
   140 NPRIME = I - 1
   145 BETA = MULT * VALU(NPRIME)
       AP = ONE
       XLMDA = ZERO
       DO 150 I = 1, NPRIME
       XMU = BETA / VALU(I)
       AP = AP * SQRT(XMU)
       XLMDA = XLMDA + B(I) ** 2
       GAMA(I) = ONE - XMU
  150 CONTINUE
       AO = AP * EXP(-XLMDA / TWO)
C
С
          DETERMINE THE DENSITY AND C.D.F. OF CENTRAL CHI-SQUARE
С
          WITH NPRIME DEGREES OF FREEDOM
С
       XN = NPRIME
       XTOP = XLIM / BETA
       N1 = NPRIME
      NN1 = 0
  160 IF (N1 .LT. 3) GOTO 180
      NN1 = NN1 + 1
      N1 = N1 - 2
      GOTO 100
  180 IF (N1 .EQ. 2) GOTO 200
      PANS = TWO * ALNORM(SQRT(XTOP), .FALSE.) - ONE
DANS = EXP(-(XTOP + ALOG(XTOP)) / TWO - CONST)
      GOTO 210
  200 PANS = EXP(-XTOP / TWO)
      DANS = PANS / TWO
      PANS = ONE - PANS
  210 IF (NN1 .LE. 0) GOTO 240
      XN1 = N1
      XN1 = XN1 / TWO - ONE
      DO 230 I = 1, NN1
      XN1 = XN1 + ONE
      DANS = DANS * XTOP / (TWO * XN1)
      PANS = PANS - TWO * DANS
  230 CONTINUE
С
С
         EVALUATE COEFFICIENTS AND HENCE DETERMINE
C
         SUCCESSIVE TERMS OF SERIES
C
  240 XN1 = XN / TWO - ONE
      NN = 0
      ANS = AO * PANS
      DNSTY = AO * DANS / BETA
      DN = DANS
      TOTAI = AO
  270 \text{ NN} = \text{NN} + 1
      COEFB(NN) = ZERO
      XNN = NN
      DO 280 J = 1, NPRIME
      BJ2NN = XNN * B(J) ** 2
```

```
COEFB(NN) = COEFB(NN) + (BJ2NN + (ONE - BJ2NN) * GAMA(J))
     * * GAMA(J) ** (NN - 1) / TWO
  280 CONTINUE
      COEFA(NN) = COEFB(NN) * AO / XNN
      IF (NN .LE. 1) GOTO 310
      ITOP = NN - 1
      DO 300 IR = 1, ITOP
      INNR = NN - IR
      COEFA(NN) = COEFA(NN) + COEFB(INNR) * COEFA(IR) / XNN
  300 CONTINUE
  310 \text{ XN1} = \text{XN1} + \text{QNE}
      DN = DN * XTOP / (TWO * XN1)
      PANS = PANS - TWO * DN
      TERM = PANS * COEFA(NN)
      TOTAI = TOTAI + COEFA(NN)
         COMPUTATION TERMINATED WHEN THE MAXIMUM POSSIBLE
С
С
         CONTRIBUTION FROM THE REMAINING TERMS IN THE SERIES
С
         EXPANSION IS LESS THAN TEST2
      IF (PANS * (ONE - TOTAI) .LT. TEST2) GOTO 340
      ANS = ANS + TERM
      DNSTY = DNSTY + COEFA(NN) * DN / BETA
      IFAULT = 5
      IF (NN' .EQ. 100) RETURN
      GOTO 270
  340 \text{ NN} = \text{NN} - 1
      IFAULT = 0
      RETURN
      END
```

Algorithm AS 107

Operating Characteristics and Average Sampling Number for a General Class of Sequential Sampling Plans

By B. LEVENTHAL

Audits of Great Britain Ltd, Ruislip, Middx.

Keywords: SEQUENTIAL SAMPLING; OPERATING CHARACTERISTICS; AVERAGE SAMPLING NUMBER

LANGUAGE

ISO Fortran

PURPOSE

This is an algorithm for calculating the operating characteristic and average sampling number functions for a wide class of closed sequential sampling plans. It is more general than Algorithm AS 67 (McPherson, 1974) at the expense of being slower and of requiring that sampling must terminate.

APPLICABLE PROBLEMS

To specify the class of sequential sampling plans to which the algorithm is applicable, we describe a sequential sampling situation and formulate a general class of closed plans that are reasonable to consider.

Suppose that a decision maker has to choose between m "terminal decisions", $d_1, d_2, \ldots d_m$, concerning an unknown scalar parameter θ . A common example is where m is 2 and the decisions correspond to the composite hypotheses " $\theta \le \theta$ *" and " $\theta > \theta$ *", where θ * is a known value. In some situations m is 3, d_1 is " $\theta \le \theta_1^*$ ", d_2 is " $\theta_1^* < \theta \le \theta_2^*$ " and d_3 is " $\theta_2^* < \theta$ ", for known θ_1^* and θ_2^* .