SELF-VALIDATED COMPUTATIONS FOR THE PROBABILITIES OF THE CENTRAL BIVARIATE CHI-SQUARE DISTRIBUTION AND A BIVARIATE F DISTRIBUTION*

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Abstract

Self-validated computations using interval analysis produce results with a guaranteed error bound. This article presents methods for self-validated computation of probabilities and percentile points of the bivariate chi-square distribution and a bivariate F distribution. For the computation of critical points (c_1, c_2) in the equation $P(Y_1 \leq c_1, Y_2 \leq c_2) = 1 - \alpha$, the case $c_1 = c_2$ is considered. A combination of interval secant and bisection algorithms is developed for finding enclosures of the percentile points of the distribution. Results are compared to previously published tables.

Keywords: Interval analysis; Guaranteed error bound; secant search

1 INTRODUCTION

When using digital computers for computations, it is wise to give some thought to error analysis of the computations. Examples of erroneous results obtained through naive computations appear often enough in scientific literature to cause concern. McCullough (1998, 1999) offers a good beginning point to this topic.

The techniques of interval analysis pioneered by Moore (1966, 1979) can provide guaranteed error bounds for the results of mathematical computations. Guaranteed error bounds, provided they are sufficiently narrow, can be used to assess the accuracy of tabled values or to evaluate the quality of results produced by scalar algorithms.

Interval analysis has been successfully utilized in statistical areas, for example Wang and Kennedy (1994), and Wright and Kennedy (2000), but has not yet had wide exposure to the statistical community. The goals of this article are (1) To present truncation error bounds for infinite series related to some bivariate chi-square and bivariate F distributions (2) To implement these bounds in calculations using interval analysis (3) To develop and apply intervalized secant methods for root-finding to the location of critical points and (4) To compare results obtained with previously published results.

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The structure of this article begins with an introduction to interval analysis in section 2 sufficient to understand the remainder of this article. Section 3 presents a new algorithm for finding guaranteed error bounds of the solution of an equation. Section 4 describes several bivariate chi-square distributions and introduces a method for obtaining guaranteed error bounds in the calculation of tables for the distribution. Section 5 takes a similar view of a bivariate F distribution. Some conclusions are stated in section 6.

2 INTERVAL ANALYSIS

Interval analysis first saw fruitful development in the 1960s, beginning with work published by Moore (1966). Since that time, interval analysis has seen extensive research for a variety of applications, for example, Hansen (1992), but has not seen wide utilization in statistical areas. This article continues the development of interval analysis applications to statistical distributions as in Wang and Kennedy (1994).

An interval $\mathbf{x}$ is defined to be a closed, bounded set of real numbers, $\mathbf{x} = [\underline{x}, \overline{x}]$. Throughout this article, boldface is used to indicate intervals. Let $\mathbf{x} = [\underline{x}, \overline{x}]$ and $\mathbf{y} = [\underline{y}, \overline{y}]$ be two intervals. The interval arithmetic operations are defined as $\mathbf{x} \circ \mathbf{y} = \{x \circ y : x \in \mathbf{x}, y \in \mathbf{y}\}$, where $\circ \in \{+, -, \cdot, /\}$ and division is undefined for $0 \in \mathbf{y}$. Interval arithmetic operations can be expressed in closed form using scalar arithmetic operations. For example, interval multiplication is defined $\mathbf{x} \cdot \mathbf{y} = [\min(\underline{x}\underline{y}, \underline{x}\overline{y}, \overline{x}\underline{y}, \overline{x}\overline{y}), \max(\underline{x}\underline{y}, \underline{x}\overline{y}, \overline{x}\underline{y}, \overline{x}\overline{y})]$. Similar expressions exist for $+, -$, and $/$. Complete details can be found in Moore (1979).

An *interval function* is defined as an interval-valued function of one or more interval arguments. A function $\mathbf{f}(\mathbf{x}_1, \ldots \mathbf{x}_n)$ is said to be an *interval extension* of the scalar function $f(x_1, \ldots, x_n)$ if $\mathbf{f}([x_1, x_1], \ldots, [x_n, x_n]) = f(x_1, \ldots, x_n)$ for all $x_i, i = 1, \ldots, n$. An interval-valued function $\mathbf{f}$ is said to be *inclusion monotonic* if $\mathbf{f}(\mathbf{x}) \subset \mathbf{f}(\mathbf{y})$ whenever $\mathbf{x} \subset \mathbf{y}$. A fundamental theorem from interval analysis states that rational interval functions are inclusion monotonic.

In this article, the *natural interval extension* of a real function will be used. This is an interval-valued function in which intervals and interval operations are substituted for scalars and scalar operations. The value of the interval extension of a function is dependent on the form of the real function. For example, let $f_1(x) = xx - 2x$ and $f_2(x) = x(x - 2)$. Let $\mathbf{f}_1$ and $\mathbf{f}_2$ be the corresponding natural interval extensions and let $\mathbf{x} = [-1, 2]$. Then $\mathbf{f}_1(\mathbf{x}) = [-6, 6]$ and $\mathbf{f}_2(\mathbf{x}) = [-6, 3]$ which both contain $[-1, 3]$, the true range of f over $\mathbf{x}$. This characteristic of interval computations to sometimes overestimate the range of a function is referred to as *interval dependency*. Attention must be given to the exact expression of a function to reduce the effect of interval dependency. Hansen (1997) discusses ways to minimize interval dependency.

When implementing interval arithmetic calculations on computers, care must also be taken to ensure that rounding errors do not invalidate the inclusion monotonicity of interval results. One way to achieve this is through the use of directed rounding modes in the floating-point calculations.

Numerical processors that are compliant with the IEEE floating-point specifications (ANSI/IEEE, 1987) can be set to round down or round up, among other modes. To maintain inclusion monotonicity during calculations, the results of a lower interval endpoint computation are always rounded down and the results of an upper interval endpoint computation are always rounded up. For example, on a hypothetical three-digit computer and using directed triangles to indicate the appropriate rounding, the real fraction $1/6$ is computed as $[1, 1]/[6, 6] = [\bigtriangledown(1/6), \bigtriangleup(1/6)] = [0.166, 0.167]$. When intervals with common decimal digits are displayed, an easily-understood representation of intervals is, for example, $[0.16^{7}_{6}]$.

Correct use of the rounding modes guarantees that the computed result contains the true value of the scalar calculation. Most rounding-mode control can be made transparent to the programmer with the aid of appropriate software packages, such as the C++ libraries BIAS (Basic Interval Arithmetic Subroutines) and PROFIL (Programmer's Optimized Fast Interval Library) developed by Knüppel (1993a,b). The calculations in this article were performed on DEC 5000 and DEC Alpha workstations with C++ and the

BIAS/PROFIL libraries.

3 INTERVAL SECANT AND BISECTION ROOT-FINDING

For a distribution function $F(x)$, the $100p^{th}$ percentile x_p is the solution of the equation $F(x_p) - p = 0$. For the bivariate distributions considered in this article, finding percentiles will involve solving the equation $P(Y_1 \leq x_p, Y_2 \leq x_p) - p = 0$, (where Y_1 and Y_2 are random variables). Intervalized Newton methods for finding zeros of functions exist and could be used. However, interval Newton methods require an interval extension of both the function being considered and its derivative, which in this case are the distribution and density functions. Using a derivative-free search algorithm eliminates the need to obtain an enclosure of the density function. It would be possible to use the technique of automatic differentiation presented in Moore (1979) to obtain an enclosure of the derivative of a function, but only at the cost of (sometimes considerable) loss of precision due to interval dependency.

A new interval algorithm for the identification of the zero of a function is now presented. The algorithm ZERO given here begins with an intervalized secant method using the Illinois modification. See Thisted (1988) for a complete explanation of this algorithm in the scalar case.

Consider the general scalar equation $F(x) = 0$ as depicted by the curved line in figure 1. Let $\mathbf{F}$ be an interval extension of F and define $\mathbf{F}(x) \equiv \mathbf{F}([x, x])$ (that is, a scalar argument x is interpreted by the interval function as the interval $[x, x]$). The algorithm begins with the specified values x_{i-1} and x_i that surround the zero of the scalar function F and satisfy $\mathbf{F}(x_{i-1}) < 0 < \mathbf{F}(x_i)$. Using an intervalized secant method, the algorithm calculates the point x_{i+1} and tries to determine if the zero of the scalar function F is to the left or the right of x_{i+1}. From this determination, either $[x_{i-1}, x_{i+1}]$ or $[x_{i+1}, x_i]$ will be used in the next iteration as the values which surround the zero of the function F. At some iteration $i + 1$ of the secant portion of the algorithm, $0 \in \mathbf{F}(x_{i+1})$ and it is not then known whether the zero of the function is to the left or the right of x_{i+1}. Figure 1 shows this condition.

The secant algorithm is successful in rapidly narrowing the enclosure of the zero of the function, but may stop while the interval is wider than desired. After the secant portion of the algorithm terminates, let

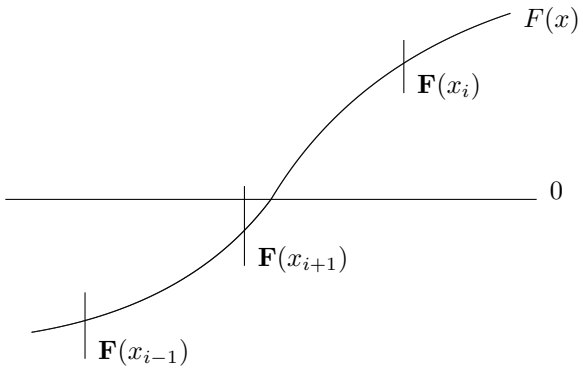

Figure 1: Termination of the secant portion of the algorithm. The curved line represents the real function and vertical line segments denote interval enclosures of the function.

$x_L = \min\{x_{i-1}, x_i\}$ and let $x_U = \max\{x_{i-1}, x_i\}$. A bisection algorithm is called twice, once each on the left $[x_L, x_{i+1}]$ and right $[x_{i+1}, x_U]$ intervals, to tighten the enclosure of the zero as much as possible, until (but not including) $0 \in \mathbf{F}(x_L), 0 \in \mathbf{F}(x_U)$. The interval $[x_L, x_U]$ is a narrow interval containing the zero of the

equation $F(x) = 0$. Figure 2 illustrates conditions at the termination of algorithm ZERO. This article uses the algorithm ZERO to calculate enclosures of the critical points of some bivariate distributions.

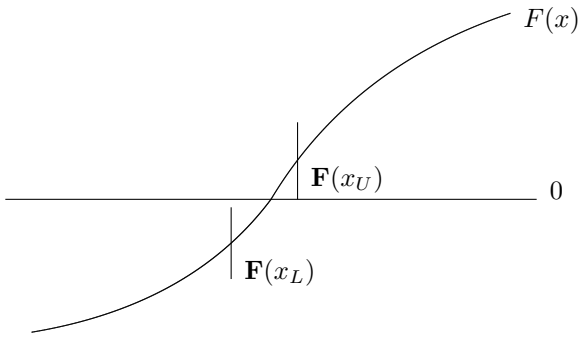

Figure 2: Termination of the bisection portion of the algorithm. The interval $[x_L, x_U]$ bounds the root of the function $F(x) = 0$.

ALGORITHM ZERO(FLOATING_POINT x_0, x_1; INTERVAL_FUNCTION $\mathbf{F}$)
REMARK Bound the root of an increasing function F. Return $[l, u]$ to user.
REMARK Check that $F(x_0) < 0 < F(x_1)$ or $F(x_1) < 0 < F(x_0)$
REMARK Bold letters denote intervals
$l := x_0$
$u := x_1$
$\mathbf{FL} := \mathbf{F}([l, l])$
$\mathbf{FU} := \mathbf{F}([u, u])$
done := FALSE
REPEAT
    $\mathbf{X}_c := u - (u - l)/(1 - \mathbf{FL}/\mathbf{FU})$ REMARK Find the secant intercept
    $x_{i+1} := (\underline{\mathbf{X}}_c + \overline{\mathbf{X}}_c)/2$ REMARK Use the midpoint for the next iterate
    $\mathbf{F}_{i+1} := \mathbf{F}([x_{i+1}, x_{i+1}])$
    IF $\underline{\mathbf{F}}_{i+1} > 0$ THEN REMARK The zero is between l and x_{i+1}
        $u := x_{i+1}$
        $\mathbf{FU} := \mathbf{F}_{i+1}$
        IF $\underline{\mathbf{F}}_i > 0$ THEN $\mathbf{FL} := \mathbf{FL}/2$ REMARK Illinois modification
    ELSE IF $\overline{\mathbf{F}}_{i+1} < 0$ THEN REMARK The zero is between x_{i+1} and u
        $l := x_{i+1}$
        $\mathbf{FL} := \mathbf{F}_{i+1}$
        IF $\underline{\mathbf{F}}_i < 0$ THEN $\mathbf{FU} := \mathbf{FU}/2$ REMARK Illinois modification
    ELSE REMARK Cannot determine if the zero is to the left or right of x_{i+1}
        done := TRUE
    IF $0 \in (\mathbf{FU} - \mathbf{FL})$ THEN
        REMARK In the next iteration, the denominator would contain zero
        done := TRUE
    $\mathbf{F}_i := \mathbf{F}_{i+1}$
UNTIL (*done* = TRUE)
REMARK Use bisection to tighten the upper endpoint

$q := l$
REPEAT
  $prevq := q$
  $prevu := u$
  $x := (q + u)/2$
  $\mathbf{FX} := \mathbf{F}([x, x])$
  IF $\underline{\mathbf{FX}} > 0$ THEN $u := x$
  ELSE IF $\overline{\mathbf{FX}} < 0$ THEN $q := l := x$
  ELSE $q := x$
UNTIL ($(q = prevq)$ AND $(u = prevu)$)
REMARK Use bisection to tighten the lower endpoint
$q := u$
REPEAT
  $prevq := q$
  $prevl := l$
  $x := (l + q)/2$
  $\mathbf{FX} := \mathbf{F}([x, x])$
  IF $\underline{\mathbf{FX}} > 0$ THEN $u := x$
  ELSE IF $\overline{\mathbf{FX}} < 0$ THEN $l := x$
  ELSE $q := x$
UNTIL ($(q = prevq)$ AND $(l = prevl)$)
RETURN $[l, u]$

4 BIVARIATE CHI-SQUARE DISTRIBUTIONS

Several applications in statistical inference utilize bivariate chi-square distributions. As mentioned by Jensen and Howe (1968), such areas include simultaneous inferences for variances, simultaneous tests in analysis of variance, simultaneous tests for goodness of fit, and the distribution of the larger of correlated chi-square variates. Gunst and Webster (1973) show how the bivariate chi-square distribution can be applied to the density function of a linear combination of independent chi-square random variables. Jensen and Jones (1969) further discuss simultaneous confidence intervals for variances while Tuprah and Woodall (1986) present a related application to bivariate dispersion quality control charts. For example, consider a manufacturing process that is characterized by two random variables, X_1 and X_2, with respective process standard deviations σ_1 and σ_2. It is desirable to detect shifts in the process standard deviations away from specified target values. If the two random variables are not independent, then the sample variances s_1^2 and s_2^2 can be used along with a region determined by a bivariate chi-square distribution to simultaneously detect shifts in the process standard deviations away from specified target values.

In general, consider two random variables with variances σ_1^2 and σ_2^2. Let s_1^2 and s_2^2 be estimates of σ_1^2 and σ_2^2 such that $\nu_i s_i^2/\sigma_i^2$ $(i = 1, 2)$ follows a chi-square distribution with ν_i degrees of freedom. The joint distribution of $\nu_1 s_1^2/\sigma_1^2$ and $\nu_2 s_2^2/\sigma_2^2$ is referred to as a bivariate chi-square distribution. Consideration will be given here to three cases of a bivariate chi-square distribution that are distinguished by degrees of freedom and the number of non-zero canonical correlations.

Case 1 In the first case, let $\{(Z_{1i}, Z_{2i}), i = 1, \ldots, m\}$ be independent random variables, $Z_{ij} \sim N(0, 1)$ with a (canonical) correlation between Z_{1i} and Z_{2i} of ρ. Then $Y_i = \sum_{j=1}^{m} Z_{ij}^2$ $(i = 1, 2)$ are chi-square random variables, each with m degrees of freedom, and with m non-zero canonical correlations ρ. The joint distribution of Y_1 and Y_2 given by Krishnaiah (1980) is

$$P[Y_1 \leq d_1, Y_2 \leq d_2] = (1 - \rho^2)^{m/2} \times$$

$$\sum_{j=0}^{\infty} \frac{\Gamma(\frac{m}{2}+j)}{j!\Gamma(\frac{m}{2})}\rho^{2j}\gamma\left(\frac{m}{2}+i,\frac{d_1}{1-\rho^2}\right)\gamma\left(\frac{m}{2}+i,\frac{d_2}{1-\rho^2}\right), \tag{1}$$

where $\gamma(\alpha,d)$ is the incomplete gamma function, $\gamma(\alpha,d)=\int_0^d x^{\alpha-1}e^{-x}/\Gamma(\alpha)\,dx$. When the infinite series in (1) is truncated after $t+1$ terms, a bound on the truncation error r_t given by Krishnaiah (1980) is

$$r_t \le 1-(1-\rho^2)^{m/2}\sum_{j=0}^{t}\frac{\Gamma(\frac{m}{2}+j)}{j!\Gamma(\frac{m}{2})}\rho^{2j}. \tag{2}$$

For completeness, the derivation of this bound is given here. Let

$$k_j=(1-\rho^2)^{m/2}\frac{\Gamma(\frac{m}{2}+j)}{j!\Gamma(\frac{m}{2})}\rho^{2j}.$$

Since $\gamma(\cdot,\cdot)\le 1$ and the k_j are the density of a Negative Binomial distribution, the truncation error r_t satisfies

$$r_t=\sum_{j=t+1}^{\infty}k_j\gamma\left(\frac{m}{2}+j,\frac{d_1}{1-\rho^2}\right)\gamma\left(\frac{m}{2}+j,\frac{d_2}{1-\rho^2}\right)\le\sum_{j=t+1}^{\infty}k_j=1-\sum_{j=0}^{t}k_j.$$

Let p_t represent the value of the series in (1) truncated after $t+1$ terms ($j=t$), and let $\mathbf{p}_t$ and $\mathbf{r}_t$ represent the natural interval extensions of p_t and r_t respectively. Then $P[Y_1\le d_1,Y_2\le d_2]=p_t+r_t\in[\underline{p}_t,\overline{p}_t+\overline{r}_t]$ for all t. The stopping value of t that is used depends on machine and software precision. In practice, $\mathbf{r}_t$ is computed successively and iteration stops when $\mathbf{r}_{t-1}=\mathbf{r}_t$ or when the width of $\mathbf{r}_t$ is less than a specified tolerance.

Case 2 Now consider the case when Y_1 and Y_2 follow chi-square distributions with m and n degrees of freedom respectively and have m non-zero canonical correlations ρ. The joint distribution of Y_1 and Y_2 given by Gunst and Webster (1973) is

$$\begin{aligned}P[Y_1\le d_1,Y_2\le d_2,] &= (1-\rho^2)^{(m+n)/2}\times\\ &\sum_{j=0}^{\infty}\sum_{k=0}^{\infty}\frac{\Gamma(\frac{m}{2}+j)}{j!\Gamma(\frac{m}{2})}\frac{\Gamma(\frac{n}{2}+k)}{k!\Gamma(\frac{n}{2})}\rho^{2(j+k)}\gamma\left(\frac{m}{2}+j,\frac{d_1}{1-\rho^2}\right)\gamma\left(\frac{n}{2}+k,\frac{d_2}{1-\rho^2}\right).\end{aligned} \tag{3}$$

Since a bound for the truncation error has not previously been published, one is given here. Because the method of derivation is completely analogous to the previous case, only the result is stated:

$$r_{t_1,t_2}\le 1-(1-\rho^2)^{m/2+n/2}\sum_{j=0}^{t_1}\sum_{k=0}^{t_2}\frac{\Gamma(\frac{m}{2}+j)}{j!\Gamma(\frac{m}{2})}\frac{\Gamma(\frac{n}{2}+k)}{k!\Gamma(\frac{n}{2})}\rho^{2(j+k)}. \tag{4}$$

Let $\mathbf{p}_{t_1,t_2}$ be the result obtained when the first (t_1+1,t_2+1) terms of the natural interval extension of (3) are used, and let $\mathbf{r}_{t_1,t_2}$ be the result obtained from the natural interval extension of (4). Then $P[Y_1\le d_1,Y_2\le d_2]=p_{t_1,t_2}+r_{t_1,t_2}\in[\underline{p}_{t_1,t_2},\overline{p}_{t_1,t_2}+\overline{r}_{t_1,t_2}]$ for all pairs (t_1,t_2).

Case 3 In the final case, Y_1 and Y_2 have chi-square distributions with $m+n$ and $m+p$ degrees of freedom, respectively, and there are m non-zero canonical correlations. The joint distribution of Y_1 and Y_2 given by Gunst and Webster (1973) is

$$\begin{aligned}P[Y_1\le d_1,Y_2\le d_2] &= (1-\rho^2)^{(m+n+p)/2}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\frac{\Gamma(\frac{m}{2}+j)}{j!\Gamma(\frac{m}{2})}\frac{\Gamma(\frac{n}{2}+k)}{k!\Gamma(\frac{n}{2})}\frac{\Gamma(\frac{p}{2}+l)}{l!\Gamma(\frac{p}{2})}\times\\ &\rho^{2(j+k+l)}\gamma\left(\frac{m}{2}+\frac{n}{2}+k+j,\frac{d_1}{1-\rho^2}\right)\gamma\left(\frac{m}{2}+\frac{p}{2}+j+l,\frac{d_2}{1-\rho^2}\right).\end{aligned} \tag{5}$$

The bound on the truncation error is again derived in a manner analogous to the first case:

$$r_t \leq 1-(1-\rho^2)^{m/2+n/2+p/2}\times \sum_{j=0}^{t_1}\sum_{k=0}^{t_2}\sum_{l=0}^{t_3}\frac{\Gamma(\frac{m}{2}+j)}{j!\Gamma(\frac{m}{2})}\frac{\Gamma(\frac{n}{2}+k)}{k!\Gamma(\frac{n}{2})}\frac{\Gamma(\frac{p}{2}+l)}{l!\Gamma(\frac{p}{2})}\rho^{2(j+k+l)}. \tag{6}$$

Similar to before, $P[Y_1 \leq d_1, Y_2 \leq d_2] \in [\underline{p}_{t_1,t_2,t_3}, \overline{p}_{t_1,t_2,t_3}+\overline{r}_{t_1,t_2,t_3}]$ for all triples (t_1,t_2,t_3) and the choice of (t_1,t_2,t_3) is determined by machine/software limitations or a tolerance level.

4.1 Computation of Tables and Numerical Results

Computing times (on DEC Alpha and DEC 5000 workstations) for a single critical point varied from a few seconds in Case 1 to a few minutes in Case 3. Subroutines to compute an enclosure of the incomplete gamma function were based on work by Wang and Kennedy (1994) and on source code by Gessner (1992).

Since the expressions (1), (3), and (5) depend on ρ only through ρ^2, tables need only include nonnegative values of ρ and need not include the trivial values of $\rho = 0$ and $\rho = 1$. For Case 1, tables 1 and 2 illustrate critical points c for $P(Y_1 \leq c, Y_2 \leq c) = 1-\alpha$ where $Y_1 \sim \chi^2(m), Y_2 \sim \chi^2(m)$. For Case 2,

Table 1: Upper 0.05 percentile points of the bivariate chi-square distribution: Case 1.

ρ	m = 2	m = 12	m = 40
0.1	7.348735242636^{94}_{62}	23.291675614644^{9}_{3}	$59.273758985599^{93}_{83}$
0.2	7.337736654468^{73}_{52}	23.279893907495^{5}_{0}	$59.258658090543^{33}_{18}$
0.3	7.318116097295^{33}_{00}	23.257752618706^{8}_{3}	$59.229809206431^{5}_{299}$
0.4	$7.287777219641^{231}_{194}$	$23.221241054104^{20}_{13}$	$59.181144305131^{6}_{290}$
0.5	7.243389878426^{35}_{03}	$23.164053099248^{80}_{72}$	59.102834933073^{5}_{11}
0.6	7.179739084402^{47}_{00}	$23.076341225205^{19}_{06}$	$58.979157192282^{6}_{782}$
0.7	7.088168635581^{74}_{21}	22.941739187792^{6}_{09}	58.783578698856^{5}_{04}
0.8	$6.952178625455^{63}_{462}$	22.729051468103^{0}_{00}	$58.465186903083^{0}_{710}$
0.9	$6.730025687074^{99}_{492}$	$22.359574679926^{3}_{195}$	$57.895406211142^{9}_{042}$

$Y_1 \sim \chi^2(m), Y_2 \sim \chi^2(m+n), n > 0$ and there are m nonzero canonical correlations. Examples of critical points c for $P(Y_1 \leq c, Y_2 \leq c) = 1-\alpha$ are given in table 3. In Case 3, $Y_1 \sim \chi^2(m+n), Y_2 \sim \chi^2(m+p), n > 0, p > 0$ and there are m nonzero canonical correlations. Table 4 illustrates critical points for this case.

The illustrative tables presented here are limited to $c_1 = c_2$ when computing the values of (c_1, c_2) in $P(Y_1 \leq c_1, Y_2 \leq c_2) = 1-\alpha$. Other schemes are possible, for example, fixing c_1 and calculating c_2, or by including a constraint. Distinct values of c_1 and c_2 can be chosen when $1-\alpha$ is the quantity to be computed.

Tables for the approximate critical points of the bivariate chi-square distribution have previously appeared in Gunst (1973), Gunst and Webster (1973), and Krishnaiah (1980). Jensen and Howe (1968) determine the probability content over select square and rectangular regions for which the marginal probabilities are specified. Dutt and Soms (1976) describe an alternative method for calculating

Table 2: Upper 0.01 percentile points of the bivariate chi-square distribution: Case 1.

ρ	m = 2	m = 12	m = 40
0.1	$10.5901634351^{801}_{788}$	$28.2909230513^{39}_{16}6$	$66.753757939^{68}_{31}61$
0.2	$10.585327860^{63}_{42}52$	$28.2868608929^{24}_{00}2$	$66.749113744^{81}_{21}75$
0.3	$10.575642698^{497}_{481}9$	$28.278218856^{28}_{04}63$	$66.739131842^{3039}_{2970}$
0.4	$10.55852476^{2011}_{1993}5$	$28.261729392^{55}_{21}28$	$66.719658957^{1106}_{0966}$
0.5	$10.529936901^{86}_{70}34$	$28.231769051^{526}_{490}9$	$66.683093898^{385}_{282}6$
0.6	$10.48358637^{91}_{68}908$	$28.178828204^{81}_{21}33$	$66.615860015^{257}_{067}6$
0.7	$10.4089856^{64}_{38}4766$	$28.086135579^{724}_{655}0$	$66.492996288^{877}_{619}3$
0.8	$10.28602680^{80}_{30}729$	$27.920471007^{549}_{418}2$	$66.263713351^{4451}_{3945}$
0.9	$10.0635917^{2077}_{1974}24$	$27.596098526^{674}_{378}8$	$65.795086198^{9439}_{8534}$

Table 3: Upper 0.05 percentile points of the bivariate chi-square distribution: Case 2.

m	$m+n$	$\rho = 0.2$	$\rho = 0.4$	$\rho = 0.6$	$\rho = 0.8$
8	10	$19.2556294984^{83}_{57}0$	$19.214557527^{118}_{051}2$	$19.117322595^{465}_{268}5$	$18.9018959^{30343}_{29502}6$
8	12	$21.4398719101^{31}_{01}9$	$21.4161617406^{314}_{243}$	$21.360410762^{626}_{459}0$	$21.243609643^{9166}_{8386}$
8	14	$23.852770931^{125}_{093}4$	$23.841241069^{155}_{085}0$	$23.814033103^{887}_{653}0$	$23.759702671^{6462}_{5233}$
8	16	$26.3613220302^{700}_{665}$	$26.3562646^{8029}_{7941}14$	$26.344214910^{737}_{417}4$	$26.32112960^{3403}_{2334}0$
8	18	$28.893827805^{94}_{57}50$	$28.891735328^{769}_{655}6$	$28.88669266^{733}_{478}61$	$28.8774013^{6245}_{4641}02$

multivariate chi-square probabilities using integral representations. The narrow interval enclosures obtained here are useful for checking the accuracy of previously tabulated values. Indeed, Table I of Gunst (1973), *Upper 100α% Critical Points*, is discovered to be widely accurate to only two decimal places (three are given), and the values in Table II, *Lower 5% Critical Points*, appear to be entirely incorrect. As noted in the text that accompanies the two tables of Gunst (1973), the critical points for $\rho = 0.10$ are nearly identical to the univariate critical points for $\alpha^* = 1 - (1 - \alpha)^{(1/2)}$. This observation holds for values obtained in this article, but does not hold for the previously published values. The values in Table 6 of Krishnaiah (1980), *Percentage Points of the bivariate chi-square distribution*, should be multiplied by two to obtain the correct values, and are then accurate to only two decimal places. If, for example, the incorrect values had been used to construct a confidence ellipsoid for the distribution of the variances of two random variables, the ellipsoid would be far too small to achieve the desired confidence.

5 A BIVARIATE F DISTRIBUTION

A multivariate F distribution, though not common, has useful applications in statistics. Schuurmann et al. (1975) point out its use in hypothesis testing under fixed-effects models, in certain two-way classification models, and in simultaneous testing of no treatment and block effects in symmetrical, balanced incomplete block designs. Tables for percentage points of a multivariate F distribution have appeared most recently in Krishnaiah (1980).

Table 4: Upper 0.05 percentile points of the bivariate chi-square distribution: Case 3.

m	n	p	$\rho = 0.4$	$\rho = 0.6$
7	1	11	$28.89212098_{6486}^{7236}$	$28.88792031_{3450}^{7461}$
6	2	12	28.89249030_{189}^{929}	$28.88907530_{39005}^{42914}$
5	3	13	$28.89284322_{3505}^{4235}$	$28.89015505_{1105}^{4641}$
4	4	14	$28.89317967_{7850}^{8563}$	$28.89115735_{1279}^{6196}$
3	5	15	$28.89349962_{8497}^{9162}$	$28.89208036_{88632}^{93269}$
2	6	16	$28.89380304_{7959}^{8769}$	$28.89292258_{0023}^{3886}$
1	7	17	$28.89408989_{8054}^{9047}$	$28.89368281_{09926}^{14038}$

The multivariate F distribution considered by Schuurmann et al. (1975) and Krishnaiah (1980) is reconsidered here. Let $S = (s_{ij})$ be a Wishart random matrix with m degrees of freedom and $E(S) = m\Sigma = m(\sigma_{ij})$. The joint distribution of $s_{11}, \ldots, s_{pp}$, the diagonal elements of S, is a multivariate χ^2 distribution with m degrees of freedom. The matrix Σ is the covariance matrix of the underlying multivariate normal random variable. Let $F_i = \frac{s_{ii}\sigma^2/m}{s^2\sigma_{ii}/n}$ $(i = 1, \ldots, p)$ where s^2/σ^2 is independently distributed as a χ^2 random variable with n degrees of freedom. Then the joint distribution of $F_1, \ldots, F_p$ is a multivariate F distribution with (m, n) degrees of freedom. When $p = 2$, $\rho = \sigma_{12}/(\sigma_{11}\sigma_{22})^{1/2}$ is the correlation between standard normal random variables that underlie the bivariate χ^2 distribution. The bivariate distribution function of F_1 and F_2, first introduced by Krishnaiah (1965), can be expressed as

$$P(F_1 \le d_1, F_2 \le d_2) = (1-\rho^2)^{m/2} \sum_{j=0}^{\infty} \frac{\Gamma(\frac{m}{2}+j)}{j!\Gamma(\frac{m}{2})} \rho^{2j} B_j \tag{7}$$

where

$$B_j = \int_0^{\infty} \frac{e^{-z/2} z^{n/2-1}}{2^{n/2}\Gamma(n/2)} I_{1j} I_{2j} dz$$

and

$$I_{kj} = \frac{1}{2^{m/2+j}\Gamma(m/2+j)} \int_0^{\frac{d_k m z}{2n(1-\rho^2)}} e^{-u/2} u^{m/2+j-1} du = \gamma\left(\frac{m}{2}+j, \frac{d_k m z}{2n(1-\rho^2)}\right) \tag{8}$$

where $\gamma(\cdot,\cdot)$ is the incomplete gamma function.

The challenging aspect of computing an interval enclosure of a critical point for the bivariate F distribution is to find an appropriate rational interval function that gives reasonably tight bounds for the enclosure of the distribution function. When the infinite series in (7) is truncated after $t+1$ terms, a bound on the truncation error r_t given by Schuurmann et al. (1975) is the same as equation (2) for the bivariate chi-square distribution. Let p_t denote the series in (7) truncated after $t+1$ terms, and let $\mathbf{p}_t$ and $\mathbf{r}_t$ denote interval enclosures of p_t and r_t respectively. Then $P[Y_1 \le d_1, Y_2 \le d_2] = p_t + r_t \in [\underline{p}_t, \overline{p}_t + \overline{r}_t]$ for all t. See section 4 for the particular t used in calculations.

To compute an enclosure for B_j via a rational interval function, ideas similar to those of Amos and Bulgren (1972) are used. The integral B_j is split into three pieces,

$$B_j = \int_0^{\infty} \cdot\, dz = \int_0^{\varepsilon_1} \cdot\, dz + \int_{\varepsilon_1}^{\varepsilon_2} \cdot\, dz + \int_{\varepsilon_2}^{\infty} \cdot\, dz, \tag{9}$$

and then the left and right tails of B_j are enclosed by the following bounds:

$$0 \leq \int_0^{\varepsilon_1} \cdot dz \leq \varepsilon_1$$

$$0 \leq \int_{\varepsilon_2}^{\infty} \cdot dz \leq 1 - \gamma\left(\frac{n}{2}, \frac{\varepsilon_2}{2}\right).$$

The middle integrand in the right-hand side of (9) covers a finite domain, over which the second derivative exists, and is computed by first-order Newton-Cotes quadrature. Some references to numerical quadrature with automatic result verification appear in Kelch (1993). The general form of Newton-Cotes quadrature is

$$\int_a^b f(x)dx = h\left[\frac{1}{2}f(a) + f(a+h) + f(a+2h) + \cdots + f(a+(m-1)h) + \frac{1}{2}f(a+hm)\right] + E \tag{10}$$

where $h = (b-a)/m$ and the error term E has the form $E = -(b-a)^3 f''(\xi)/12m^2$ for some $\xi \in (a,b)$. The interval extension of E involves the computation of the interval enclosure of the second derivative of f, $\mathbf{f}''([a,b])$. If f'' is a rational function, as in this problem, then the interval extension $\mathbf{f}''$ is inclusion monotonic and the width of $\mathbf{f}''([a,b])$ is likely to be greater than $\mathbf{f}''([a',b'])$ for $[a',b'] \subset [a,b]$. Minimizing the width of the error term is one of the steps in achieving highly accurate final results. For this reason, the middle integral in the right-hand side of (9) is actually computed as the sum of a series of subintegrals, each of which is evaluated by numerical quadrature:

$$\int_{\epsilon_1}^{\epsilon_2} \cdot dz = \int_{\epsilon_1}^{\epsilon_1+\nu} \cdot dz + \int_{\epsilon_1+\nu}^{\epsilon_1+2\nu} \cdot dz + \cdots + \int_{\epsilon_1+(k-1)\nu}^{\epsilon_1+k\nu} \cdot dz + \int_{\epsilon_1+k\nu}^{\epsilon_2} \cdot dz. \tag{11}$$

Tuning the numerical integration parameters $(\epsilon_1, \epsilon_2, k, \nu, h, m)$ of the method used here is not a straightforward matter. Generally speaking, increasing the number of quadrature points will increase the accuracy (narrowness) of the final interval answer. A limit is reached, however, when increasing the number of quadrature points becomes counter-productive. This happens because each interval function evaluation at a quadrature point results in a slight amount of overestimation and underestimation of the true value. Increasing m results in a narrower enclosure of the error E for each integrand, but eventually this gain is nullified by the sum of the overestimated and underestimated function values. A similar phenomenon occurs in deciding how many subintegrals to use in evaluating $\int_{\epsilon_1}^{\epsilon_2} \cdot dz$. Experimentation was used to select appropriate values for $\epsilon_1, \epsilon_2, k, \nu, h$ and m.

To achive the greatest possible accuracy, a hand-derived expression for f'' was coded into the software instead of using automatic differentiation. The resulting expression involves evaluation of the term $x^{m/2-2}$ over an interval with a lower endpoint of 0. This limits the degrees of freedom to $m \geq 5$.

5.1 Computation of Tables and Numerical Results

Krishnaiah (1980) actually gives expressions for probability integrals over arbitrary rectangular regions, $P(c_1 \leq F_1 \leq d_1, c_2 \leq F_2 \leq d_2)$, but in all previously published tables of critical points, $c_1 = c_2 = 0$. Herein, tables of critical points d were computed for $P(F_1 \leq d, F_2 \leq d) = \alpha$. The computation of self-validated critical points for this bivariate F distribution is computationally intensive. The probability content of a rectangular region can be computed in a few minutes, but this is likely to be prohibitively costly for implementation of real-time computation of critical points. Since determination of critical points involves finding the roots of an equation, each *entry* in tables 5 and 6 required several hours to compute on a DEC 5000 workstation. Less time would be required for wider enclosures. For the bivariate F distribution, the

real utility of interval analysis is the guarantee of accuracy and verification of previously published tables. The tables published in Schuurmann et al. (1975) and Krishnaiah (1980) are generally quite accurate, but do have slight errors in the last (hundredths) digit that are likely due to rounding, exactly the kind of error that interval analysis can eliminate. Tables 5 and 6 illustrate the accuracy achieved by the software developed for this research.

Table 5: Upper 0.05 percentile points of the bivariate F distribution.

	$n = 10$			
m	$\rho = 0.1$	$\rho = 0.3$	$\rho = 0.5$	$\rho = 0.7$
2	5.31734^{58}_{16}	5.2768^{13}_{08}	5.18758^{96}_{74}	5.02529^{78}_{34}
4	4.3110^{81}_{77}	4.28342^{36}_{02}	4.22239^{63}_{28}	4.11107^{52}_{12}
6	3.89658^{81}_{49}	3.87377^{47}_{14}	3.82350^{55}_{20}	3.73205^{79}_{38}
8	3.66318^{49}_{34}	3.64307^{81}_{48}	3.59884^{95}_{59}	3.51864^{45}_{01}
10	3.51093^{94}_{60}	3.49262^{99}_{65}	3.4524^{23}_{18}	3.37971^{84}_{35}

Table 6: Upper 0.01 percentile points of the bivariate F distribution.

	$n = 10$			
m	$\rho = 0.1$	$\rho = 0.3$	$\rho = 0.5$	$\rho = 0.7$
2	9.3014^{99}_{81}	9.2532^{24}_{09}	9.1430^{61}_{46}	8.9312^{17}_{01}
4	7.1869^{98}_{87}	7.1526^{70}_{58}	7.0749^{36}_{24}	6.9271^{94}_{83}
6	6.3616^{99}_{77}	6.3325^{93}_{83}	6.26714^{96}_{03}	6.1440^{67}_{58}
8	5.9094^{83}_{61}	5.8833^{28}_{19}	5.8248^{23}_{14}	5.7156^{75}_{66}
10	5.6197^{60}_{38}	5.5955^{96}_{87}	5.5417^{56}_{47}	5.4419^{38}_{29}

6 CONCLUSIONS

The tables that appear in this article are included to demonstrate the very high precision and the guarantee of accuracy that are obtained via the use of interval analysis. Except in certain cases, the use of more digits in the table than significant digits in available data should be discouraged. The great value of such high-quality numbers is more likely in knowing that the second digit of a critical point is guaranteed to be accurate than in knowing what the eighth digit is. These tables can also be used to assess the quality of scalar algorithms.

Even in algorithms where theoretical error analysis provides a bound for error terms, computer arithmetic rounding and cancellation errors can have catastrophic effects. In this article, interval analysis techniques have been successfully applied to bivariate chi-square distributions and a bivariate F distribution to produce tables of critical points with guaranteed error bounds. The results obtained revealed inaccuracies and limitations of some earlier published tables and verified the accuracy of other tables. While correct tables are useful in and of themselves, this research also provides new methodologies

for implementing self-verified computations in a statistical context. Further research in the areas of interval analysis in statistical problems should produce fruitful results.

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References

Amos, D. E. and Bulgren, W. G. (1972). Computation of a Multivariate F Distribution. *Mathematics of Computation*, 26(117):255–264.

ANSI/IEEE (1987). A Radix-Independent Standard for Floating-Point Arithmetic. ANSI/IEEE Standard 854-1987. 9

Dutt, J. E. and Soms, A. P. (1976). An Integral Representation Technique for Calculating General Multivariate Probabilities with an Application to Multivariate χ^2. *Communications in Statistics–Theory and Methods*, 5:377–388. 2

Gessner, M. (1992). Self-Validating Computations of Standard Normal and Incomplete Gamma Probabilities. Master's thesis, Iowa State University. 7

Gunst, R. F. (1973). On Computing Critical Points for a Bivariate Chi-Square Random Variable. *Communications in Statistics*, 2:221–224. 7

Gunst, R. F. and Webster, J. T. (1973). Density Functions of the Bivariate Chi-Square Distribution. *Journal of Statistical Computation and Simulation*, 2:275–288. 7, 8

Hansen, E. (1992). *Global Optimization Using Interval Analysis*. Marcel Dekker, New York. 5, 6, 7

Hansen, E. (1997). Sharpness in Interval Computations. *Reliable Computing*, 3:17–29. 2

Jensen, D. R. and Howe, R. B. (1968). Probability Content of the Bivariate Chi-Square Distribution Over Rectangular Regions. *Virginia Journal of Science*, 19:233–239. 2

Jensen, D. R. and Jones, M. Q. (1969). Simultaneous Confidence Intervals for Variances. *Journal of the American Statistical Association*, 64:324–332. 5, 7

Kelch, R. (1993). Numerical Quadrature by Extrapolation with Automatic Result Verification. In Adams, E. and Kulisch, U., editors, *Scientific Computing with Automatic Result Verification*, pages 143–185. Academic Press, New York. 5

Knüppel, O. (1993a). BIAS – Basic Interval Arithmetic Subroutines. Technical Report 93.3, Informationstechnik, Technische Uni. Hamburg–Harburg. 10

Knüppel, O. (1993b). PROFIL – Programmer's Runtime Optimized Fast Interval Library. Technical Report 93.4, Informationstechnik, Technische Uni. Hamburg–Harburg. 2

Krishnaiah, P. R. (1965). On the Simultaneous ANOVA and MANOVA Tests. *Annals of the Institute of Statistical Mathematics*, 17:35–53. 2

Krishnaiah, P. R. (1980). *Handbook of Statistics, Vol. 1*, chapter Computations of Some Multivariate Distributions, pages 745–971. North-Holland Publishing Company, New York. 9

McCullough, Bruce D. (1998). Assessing the Reliability of Statistical Software: Part I. *The American Statistician*, 52:355–363. 5, 6, 7, 8, 9, 10, 11

McCullough, Bruce D. (1999). Assessing the Reliability of Statistical Software: Part II. *The American Statistician*, 53:149–159. 1

Moore, R. E. (1966). *Interval Analysis*. Prentice-Hall, Englewood Cliffs, N.J. 1

Moore, R. E. (1979). *Methods and Applications of Interval Analysis*. SIAM, Philadelphia. 1, 2

Schuurmann, F. J., Krishnaiah, P. R., and Chattopadhyay, A. K. (1975). Tables for a Multivariate F Distribution. *Sankhya*, 37:308–331. 1, 2, 3

Thisted, R. A. (1988). *Elements of Statistical Computing*. Chapman and Hall, New York. 8, 9, 11

Tuprah, K. and Woodall, W. H. (1986). Bivariate Dispersion Quality Control Charts. *Communications in Statistics – Simulation and Computing*, 15:505–522. 3

Wang, M. C. and Kennedy, W. J. (1994). Self-Validating Computations of Probabilities for Selected Central and Noncentral Univariate Probability Functions. *Journal of the American Statistical Association*, 89:878–887. 5

Wright, K. and Kennedy, W. J. (2000). An Interval Analysis Approach to the EM Algorithm. *Journal of Computational and Graphical Statistics*, 9:303–318. 1, 2, 7

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