

**CALCULATION OF UPPER TAIL PERCENTILES FOR  
THE CHI-SQUARE DISTRIBUTION**

**BY  
HERMAN RUBIN and JAMES V. ZIDEK**

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CALCULATION OF UPPER TAIL PERCENTILES FOR THE  
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1. Summary

This report describes a procedure for determining upper tail percentiles of the chi-square distribution with an arbitrary number of degrees of freedom. It consists of two main parts. The first is a description of an effective iterative technique, which is to be published by H. Rubin, for solving equations of the form  $f(x) = 0$ , given the feasibility of computing  $f$  and its derivatives. The second, in the application of this technique to the chi-square distribution, is the continued fraction approximation to the tail integral of the chi-square density function. An alternative procedure is given for the cases in which the sequence of approximants to this continued fraction converge slowly.

2. Iterative Solution of  $f(x) = 0$ .

In general, let  $f(x)$  denote a real valued function defined on the real line. Suppose  $f$  can be represented as a power series, that is,

$$(1) \quad f(x+y) = \sum_{n=0}^{\infty} a_n(x) y^n,$$

where  $a_n(x) = f^{(n)}(x)/n!$

In the problem with which this report is concerned, we are interested in solving equations of the form,

$$(2) \quad f(x) = 0 .$$

Suppose  $x_0$  is an initial approximation to the required solution. If  $x'$  denotes this solution, let

$$x' - x_0 = (t + \gamma t^2) / (1 - \alpha t - \beta t^2) ,$$

where  $\alpha$ ,  $\beta$ , and  $\gamma$  are constants chosen in accordance with the following considerations.

Using equation (1), we have

$$(3) \quad (1 - \alpha t - \beta t^2) f\left(x_0 + \frac{t + \gamma t^2}{1 - \alpha t - \beta t^2}\right) = \sum_{n=0}^{\infty} a_n(x_0) \frac{(t + \gamma t^2)^n}{(1 - \alpha t - \beta t^2)^{n-1}} .$$

If  $\alpha$ ,  $\beta$ , and  $\gamma$  are chosen so that  $(\alpha, \beta, \gamma)$  is one of the solutions of the equations

$$(4) \quad \begin{aligned} & 2\gamma + \alpha + a_3(x_0)/a_2(x_0) = 0 \\ & \alpha^2 + \gamma^2 + 2\alpha\gamma + \beta + 3\gamma a_3(x_0)/a_2(x_0) + \\ & 2\alpha a_3(x_0)/a_2(x_0) + a_4(x_0)/a_2(x_0) = 0 , \end{aligned}$$

it is easily shown that the coefficients of  $t^3$  and  $t^4$  on the right hand side of equation (3) vanish while that of  $t^5$  becomes  $2a_3^3(x_0)/a_2^2(x_0) - 3a_3(x_0)a_4(x_0)/a_2(x_0) + a_5(x_0)$ . Let  $(\alpha_0, \beta_0, \gamma_0)$  denote a solution of equations (4). Then an approximation,  $t_0$ , to the value of  $t$  for which

$$x' - x_0 = (t + \gamma_0 t^2) / (1 - \alpha_0 t - \beta_0 t^2) ,$$

is the smaller solution, in absolute value, of

$$(1 - \alpha_0 t - \beta_0 t^2) f(x_0) + f^{(1)}(x_0)(t + \gamma_0 t^2) + \frac{1}{2} f^{(2)}(x_0) t^2 = 0 ,$$

that is,

$$t_0 = 2f(x_0) [\alpha_0 f(x_0) - f^{(1)}(x_0)] \pm \{ (\alpha_0^2 + 4\beta_0) f^2(x_0) - 2(2\gamma_0 + \alpha_0) f^{(1)}(x_0) f(x_0) + (f^{(1)}(x_0))^2 - 2f(x_0) f^{(2)}(x_0) \}^{\frac{1}{2}}^{-1},$$

where the plus or minus sign is chosen according as  $\alpha_0 f(x_0) - f^{(1)}(x_0)$  is positive or negative.

Let  $x_1 = x_0 + (t_0 + \gamma_0 t_0^2) / (1 - \alpha_0 t_0 - \beta_0 t_0^2)$ . Then  $x_1$  is an improved approximation of  $x'$ . Define a sequence,  $\{x_n\}$ , of successive approximations of  $x'$ , by the relation

$$x_n = x_{n-1} + (t_{n-1} + \gamma_{n-1} t_{n-1}^2) / (1 - \alpha_{n-1} t_{n-1} - \beta_{n-1} t_{n-1}^2) \quad (n = 1, 2, \dots)$$

where  $(\alpha_{n-1}, \beta_{n-1}, \gamma_{n-1})$  is one of the solutions of equations (4) and

$$(5) \quad t_{n-1} = 2f(x_{n-1}) [\alpha_{n-1} f(x_{n-1}) - f^{(1)}(x_{n-1})] \pm \{ (\alpha_{n-1} f(x_{n-1}) - f^{(1)}(x_{n-1}))^2 - 4f(x_{n-1}) (\gamma_{n-1} f^{(1)}(x_{n-1}) - \beta_{n-1} f(x_{n-1}) + \frac{1}{2} f^{(2)}(x_{n-1})) \}^{\frac{1}{2}}^{-1}$$

the plus or minus sign being chosen according as  $\alpha_{n-1} f(x_{n-1}) - f^{(1)}(x_{n-1})$  is positive or negative.

### 3. Computation of Percentiles of the Chi-Squared Distribution (p small).

The procedure just described can be applied to the problem of computing upper tail percentiles for the chi-squared distribution with  $k(k=1, 2, \dots)$  degrees of freedom. Let  $X^2(k)$  denote the random variable having a chi-squared distribution with  $k$  degrees of freedom, and  $X_p^2(k)$ , the  $(1-p)^{\text{th}}$  percentile for this distribution. Then  $X^2(k)$

has probability density function

$$g_{X(k)}(x)dx = 2^{-k/2} \Gamma^{-1}(k/2) x^{k/2-1} e^{-x/2} dx \quad (x > 0)$$

$$= 0 \quad (x \leq 0).$$

If we let  $y(k) = X^2(k)/2$ ,  $y(k)$  has probability density function

$$g_{y(k)}(x)dx = \Gamma^{-1}(k/2) x^{k/2-1} e^{-x} dx \quad (x > 0)$$

$$= 0 \quad (x \leq 0),$$

that is,  $y(k)$  has the gamma distribution with parameter  $k/2$ . If  $y_p(k)$  denotes the  $(1-p)^{\text{th}}$  percentile for this distribution,

$$(6) \quad X_p^2(k) = 2y_p(k).$$

For simplicity, we determine  $y_p(k)$  using the procedure described in section 2, and  $X_p^2(k)$  is then obtained using equation (6).

To this end, let

$$f(x) = \log_e \left\{ \frac{1}{\Gamma(k/2)} \int_x^\infty e^{-t} t^{k/2-1} dt \right\} - \log_e p, \quad (0 < p < 1).$$

Then, if  $g(x)$  and  $h(x)$  denote  $-e^{-x} x^{k/2-1}$  and  $\int_x^\infty e^{-t} t^{k/2-1} dt$ , respectively,

$$(7) \quad \begin{aligned} f^{(1)} &= g/h \\ f^{(2)} &= h^{-1} [g^{(1)} - g \{ \frac{g}{h} \}] \\ f^{(3)} &= h^{-1} [g^{(2)} - 3g^{(1)} \{ \frac{g}{h} \} + 2g \{ \frac{g}{h} \}^2] \\ f^{(4)} &= h^{-1} [g^{(3)} - 4g^{(2)} \{ \frac{g}{h} \} - 3(g^{(1)})^2/h + 12g^{(1)} \{ \frac{g}{h} \}^2 - 6g \{ \frac{g}{h} \}^3]. \end{aligned}$$

Note that in the computation of these derivatives significant figures will be lost through cancellation.

Now, using the even part of expansion (92.9) given by Wall [1, page 356],

$$(8) \quad h(x) = \frac{e^{-x} x^{\frac{k}{2}}}{x+1-\frac{k}{2}+\frac{(\frac{k}{2}-1) \cdot 1}{x+3-\frac{k}{2}+\frac{(\frac{k}{2}-2) \cdot 2}{x+5-\frac{k}{2} + \dots}}$$

Table 1 in the appendix is comprised of calculations which indicate the rate at which the sequence of successive approximants to  $h(x)$  converges. When  $p$  is moderate and  $k$  is large, this convergence is slow. Therefore, it is preferable, in these cases, to use the alternate procedure, for the calculation of  $\chi_p^2(k)$ , described in Section 4 of this report.

At the same time,

$$(9) \quad g^{(1)}(x) = -g(x) \left( \frac{x-\frac{k}{2}+1}{x} \right)$$

$$g^{(2)}(x) = g(x) \left[ \left( \frac{x-\frac{k}{2}+1}{x} \right)^2 - \frac{(\frac{k}{2}-1)}{x} \right]$$

$$g^{(3)}(x) = -g(x) \left[ \left( \frac{x-\frac{k}{2}+1}{x} \right)^3 - \frac{3(\frac{k}{2}-1)}{x^2} \left( \frac{x-\frac{k}{2}+1}{x} \right) - \frac{2(\frac{k}{2}-1)}{x^3} \right].$$

For the initial estimate,  $x_0$ , we take, using the Hilferty-Wilson approximation (cf., Kendall and Stuart, [2], page 373)

$$(10) \quad x_0 = k \left[ 2^{\frac{2}{3}} \left( \frac{1}{2} - \frac{1}{9k} \right) + z_p \left( \frac{2^{\frac{1}{3}}}{9k} \right)^{\frac{1}{2}} \right]^3,$$

where  $z_p$  is defined by

$$\frac{1}{\sqrt{2\pi}} \int_{z_p}^{\infty} e^{-t^2/2} dt = p,$$

and may be obtained, with a high degree of accuracy, using, for example, tables provided by the National Bureau of Standards [3].

Kendall and Stuart ([2], page 374) give a table containing calculated values of  $x_0$  for several values of  $p$  and  $k$ . For example, they give for  $k = 42$ , the values 29.060 and 33.113 for  $p = 0.05$  and  $p = 0.01$ , while for  $k = 82$ , 52.068 and 57.355 are given for  $p = 0.05$  and  $p = 0.01$ . These compare favorably with the correct values of 29.063, 33.103, 52.069, and 57.347, respectively.

A summary of the procedure is given below. It should be noted that by choosing

$$(11) \quad \begin{aligned} \alpha_n &= 0 \\ \gamma_n &= -\frac{1}{6} f^{(3)}(x_n)/f^{(2)}(x_n) \\ \beta_n &= -\frac{1}{12} f^{(4)}(x_n)/f^{(2)}(x_n) + \frac{5}{36} [f^{(3)}(x_n)/f^{(2)}(x_n)]^2, \end{aligned}$$

( $n=0,1,2,\dots$ ), some computational simplifications occur.

With  $p$  and  $k$  specified, find  $z_p$  and  $x_0$  using equation (10). Having determined  $x_{n-1}$  ( $n=1,2,\dots$ ), compute  $f(x_{n-1})$  and  $f^{(i)}(x_{n-1})$  ( $i=1,2,3,4$ ) using representation (8) and equations (7), respectively. Calculate  $\alpha_{n-1}, \beta_{n-1}$ , and  $\gamma_{n-1}$ . Then compute  $t_{n-1}$  using equation (5).



If the values suggested in equations (11) are used, we have

$$(12) \quad t_{n-1} = -2f(x_{n-1})[f^{(1)}(x_{n-1}) - \{4(\beta_{n-1}f^2(x_{n-1}) - \gamma_{n-1}f^{(1)}(x_{n-1})f(x_{n-1})) + (f^{(1)}(x_{n-1}))^2 - 2f(x_{n-1})f^{(2)}(x_{n-1})\}^{\frac{1}{2}} - 1].$$

Finally,

$$x_n = x_{n-1} + (t_{n-1} + \gamma_{n-1}t_{n-1}^2) / (1 - \alpha_{n-1}t_{n-1} - \beta_{n-1}t_{n-1}^2).$$

In this way, a sequence,  $\{x_i\}$ , of successive approximations is obtained. The calculations are complete when the prescribed degree of accuracy is attained.

Now, if the last member of this sequence is denoted by  $y_p(k)$ , the  $(1-p)^{\text{th}}$  percentile for the chi-square distribution with  $k$  degrees of freedom is, to the prescribed degree of accuracy,

$$\chi_p^2(k) = 2y_p(k).$$

This procedure, using the values suggested in equation (11) is illustrated in Table 2.

#### 4. Alternate Method for Computation of $\chi_p^2(k)$ (medium $p$ , large $k$ ).

As was pointed out in Section 3 it is difficult to apply the iterative method of that section because the continued fraction approximation to the integral converges slowly when  $p$  is moderate and  $k$  is large. In this section, we describe an alternate method suitable for the calculation of  $\chi_p^2(k)$  in these cases.

Define a random variable,  $T_k$  by

$$(v^{1/3} + \frac{1}{3} T_k v^{-1/6})^3 = y(k),$$

where  $v = k/2 - 1/3$  and  $y(k)$  denotes the random variable having the gamma distribution with parameter  $k/2$ . Then  $T_k$  has density

$$(13) \quad f_{T_k}(t) = \frac{v^{-1/6}}{\Gamma(v+1/3)} e^{-(v^{1/3} + \frac{1}{3} t v^{-1/6})^3} (v^{1/3} + \frac{1}{3} t v^{-1/6})^{3v} \quad (0 < t < (\infty),$$

where, for convenience, the subscript,  $k$  on  $T_k$  has been suppressed.

Using the asymptotic expansion (cf. Whittaker and Watson, [4], page 252),

$$\log \Gamma(x) = (x - \frac{1}{2}) \log x - x + \frac{1}{2} \log(2\pi) + \frac{1}{12x} - \frac{1}{360x^3} + \dots,$$

we obtain

$$f_{T_k}(t) \sim \phi(t) \left(1 + \frac{1}{36v} + \frac{17}{2592v^2} + \dots\right) \left(1 - \frac{t^4}{108v} + \frac{t^5}{405v^{3/2}} + \frac{1}{v^2} \left[\frac{t^8}{23328} - \frac{t^6}{1458}\right] + \frac{1}{v^{5/2}} \left[\frac{t^7}{5103} - \frac{t^9}{43740}\right] + \dots\right),$$

where  $\phi(t) = e^{-t^2/2} / \sqrt{2\pi}$ . Thus

$$(14) \quad \int_{\xi}^{\infty} f_{T_k}(t) dt \sim N_0(\xi) + \frac{1}{v} \left[ \frac{1}{36} N_0(\xi) - \frac{1}{108} N_4(\xi) \right] + \frac{1}{v^{3/2}} \left[ \frac{N_5(\xi)}{405} \right] + \frac{1}{v^2} \left[ \frac{17 N_0(\xi)}{2592} - \frac{N_4(\xi)}{3888} - \frac{N_6(\xi)}{1458} + \frac{N_8(\xi)}{23328} \right] + \frac{1}{v^{5/2}} \left[ \frac{N_5(\xi)}{14580} + \frac{N_7(\xi)}{5103} - \frac{N_9(\xi)}{43740} \right] + \dots,$$

where

$$N_r(\xi) = \frac{1}{\sqrt{2\pi}} \int_{\xi}^{\infty} e^{-\frac{t^2}{2}} t^r dt \quad (r=1,2,\dots).$$

If we denote the coefficient of  $(v^{-1/2})^j$  ( $j=2,3,\dots$ ), in expansion (14), by  $G_j(\xi)$  and expand  $\int_{\xi}^{\infty} f_T(t)dt$  about  $z_p$ , we obtain,

$$(15) \quad \int_{\xi}^{\infty} f_T(t)dt = p + \sum_{n=2}^{\infty} v^{-n/2} G_n(z_p) + (N'_0(z_p) + \sum_{n=2}^{\infty} v^{-n/2} G'_n(z_p)) \\ \times (\xi - z_p) + \frac{1}{2} (N''_0(z_p) + \sum_{n=2}^{\infty} v^{-n/2} G''_n(z_p)) (\xi - z_p)^2 + \dots$$

Let

$$R(z_p, v) = z_p + \sum_{n=2}^{\infty} v^{-n/2} c_n(z_p)$$

where the  $\{c_i\}_{i=2}^{\infty}$  are chosen so that

$$\int_{R(z_p, v)}^{\infty} f_T(t)dt = p$$

for all  $v$ , that is, to make  $R(z_p, v)$  the  $(1-p)^{th}$  percentile for the random variable whose density is given by equation (13). It is easily verified that

$$c_2 = G_2(z_p)/\phi(z_p), \quad c_3 = G_3(z_p)/\phi(z_p),$$

$$c_4 = \phi^{-1}(z_p) [G_4(z_p) + c_2 G'_2(z_p) + \frac{1}{2} c_2^2 \phi(z_p) z_p],$$

$$c_5 = \phi^{-1}(z_p) [G_5(z_p) + c_3 G'_2(z_p) + c_2 G'_3(z_p) + c_2 c_3 z_p \phi(z_p)]$$

Upon application of the relations,  $N_r(z) = \phi(z) z^{r-1} + (r-1) N_{r-2}(z)$  and

$N_r'(z) = -z^r \phi(z)$  ( $r=1,2,\dots$ ), and simplification we obtain

$$c_2 = -\frac{1}{108} (z_p^3 + 3z_p) \quad c_3 = \frac{1}{405} (z_p^4 + 4z_p^2 + 8)$$

$$c_4 = -\frac{1}{2592} (z_p^5 + 4z_p^3 + 15z_p)$$

$$c_5 = \frac{1}{76545} (z_p^6 - 15z_p^4 - 18z_p^2 + 48).$$

Finally, the required percentile for the chi-square distribution with  $k$  degrees of freedom is

$$\chi_p^2(k) = 2(v^{1/3} + \frac{1}{3} R(z_p, v)v^{-1/6})^3,$$

using equation (6) and since

$$y_p(k) = (v^{1/3} + \frac{1}{3} R(z_p, v)v^{-1/6})^3.$$

Calculations, using the approximation,

$$R(z_p, v) \approx z_p + c_2 v^{-1} + c_3 v^{-3/2} + c_4 v^{-2} + c_5 v^{-5/2}$$

yielded, in the cases  $k = 30$  and  $P = 0.1, 0.01, 0.001$ , the tabulated values for  $\chi^2$ , of 40.2560, 50.892, and 59.703, respectively.

APPENDIX

Table 1.

Successive approximations,

$$D_n = \frac{e^{-x} x^{k/2}}{x+1-k/2} \dots + \frac{[k/2-(n-1)](n-1)}{x+(2n-1)-k/2},$$

to  $h(x)$  for various values of  $x$  and several successive integers  $n$  and  $k = 5$ .

	$n$	$D_n$
$x=40$	1	0.1116631751 (-15)
	2	0.1105992097 (-15)
	3	0.1105998181 (-15)
	4	0.1105998186 (-15)
	5	0.1105998186 (-15)
$x=10$	1	0.168902569 (-2)
	2	0.166110791 (-2)
	3	0.1661315547 (-2)
	4	0.1661317266 (-2)
	5	0.1661317311 (-2)
	6	0.1661317313 (-2)
	7	0.1661317313 (-2)
$x=5$	1	0.1076179107
	2	0.0998383026
	3	0.1000094174
	4	0.1000130146
	5	0.1000132282
	6	0.1000132401
	7	0.1000132506
	8	0.1000132509

Table 2.

Calculations illustrating the use of the procedure described in Section 3. Here  $k = 6$ ,  $p = 10^{-15}$ ,  $z_p \approx 7.94$  and  $x_0 = 46.4$ .

$f(x_0)$	= -4.83668 06556 61	$\alpha_0 = 0$
$f^{(1)}(x_0)$	= -0.95782 46788	$\gamma_0 = 0.00702 29602 0$
$f^{(2)}(x_0)$	= -0.00088 89830 100	$\beta_0 = 0.00002 47601 2325$
$f^{(3)}(x_0)$	= 0.00003 74597 5383	$t_0 = -5.15496 3915$
$f^{(4)}(x_0)$	= -0.00000 23666 47654	$x_1 = 41.42839 064$
$f(x_1)$	= -0.08657 06189 89	$\alpha_1 = 0$
$f^{(1)}(x_1)$	= -0.95288 79229	$\gamma_1 = 0.00784 32843 50$
$f^{(2)}(x_1)$	= -0.00110 91574 19	$\beta_1 = 0.00003 09130 1835$
$f^{(3)}(x_1)$	= 0.00005 21966 2219	$t_1 = -0.09092 02279$
$f^{(4)}(x_1)$	= -0.00000 36824 80654	$x_2 = 41.33753 504$
$f(x_2)$	= $6.1 \times 10^{-9}$ *	

\* At this stage, the error,  $x' - x_2$ , is approximately  $f(x_2)$ . Thus

$$x_p^2(6) \approx 82.67507008,$$

with  $p = 10^{-15}$ .

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