CALCULATION OF UPPER TAIL PERCENTILES FOR
THE CHI-SQUARE DISTRIBUTION

BY
HERMAN RUBIN and JAMES V. ZIDEK

TECHNICAL REPORT NO. 102
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DEPARTMENT OF STATISTICS
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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) \[ f(x) = 0. \]

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

\[
x' - x_0 = \frac{(t+\gamma t^2)}{(1-\alpha t - \beta t^2)},
\]

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

Using equation (1), we have

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

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

(4) \[
\begin{align*}
2\gamma + \alpha + \frac{a_2(x_0)}{a_2(x_0)} &= 0, \\
\alpha^2 + \gamma^2 + 2\alpha \gamma + \beta + \frac{a_3(x_0)}{a_2(x_0)} &= 0,
\end{align*}
\]

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

\[
2a_3(x_0)/a_2(x_0) - 3a_3(x_0)a_4(x_0)/a_2(x_0) + a_5(x_0).\]

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

\[
x' - x_0 = \frac{(t+\gamma_0 t^2)}{(1-\alpha_0 t - \beta_0 t^2)},
\]

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,

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

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

\[
x_n = x_{n-1} + (t_n - \gamma_n n_1 - \beta_n n_1^2)/(1 - \alpha_n t_n - \beta_n t_n^2)(n = 1, 2, \ldots)
\]

where \((\alpha_n, \beta_n, \gamma_n)\) is one of the solutions of equations (4) and

\[
t_n = 2f(x_{n-1})[\alpha_n f(x_{n-1}) - f^{(1)}(x_{n-1})] + [(\alpha_n f(x_{n-1}) - f^{(1)}(x_{n-1})^2
- 4f(x_{n-1})(\gamma_n f^{(1)}(x_{n-1}) - \beta_n f(x_{n-1}) + \frac{1}{2} f^{(2)}(x_{n-1}))^2]^{-1}
\]

the plus or minus sign being chosen according as \(\alpha_n f(x_{n-1}) - f^{(1)}(x_{n-1})\) 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 \(k(k+1,2,\ldots)\) degrees of freedom. Let \(X^2(k)\) denote the random variable having a chi-squared distribution with \(k\) degrees of freedom, and \(X^2_p(k)\), the \((1-p)^{th}\) percentile for this distribution. Then \(X^2_p(k)\)
has probability density function
\[
g_2 \frac{x}{x(k)} (x) dx = 2^{-k/2} \Gamma^{-1}(k/2)x^{k/2-1}e^{-x/2} dx \quad (x > 0)
\]
\[
= 0 \quad (x \leq 0).
\]

If we let \( y(k) = x^2(k)/2 \), \( y(k) \) has probability density function
\[
g_y(y(k)) dx = \Gamma^{-1}(k/2)x^{k/2-1}e^{-x} dx \quad (x > 0)
\]
\[
= 0 \quad (x \leq 0),
\]
that is, \( y(k) \) has the gamma distribution with parameter \( k/2 \). If \( y_p(k) \) denotes the \((1-p)^{th}\) percentile for this distribution,
\[
(6) \quad \chi_p^2(k) = 2y_p(k).
\]

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

To this end, let
\[
f(x) = \log e \left\{ \frac{1}{\Gamma(k/2)} \int_x^\infty e^{-t} t^{k/2-1} dt \right\} - \log e \quad p, \quad (0 < p < 1).
\]

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,
\[
(7) \quad f(1) = g/h
\]
\[
f(2) = h^{-1}[g(1) - g(\frac{k}{h})]
\]
\[
f(3) = h^{-1}[g(2) - 3g(1)g(\frac{k}{h}) + 2g(\frac{k}{h})]^2]
\]
\[
f(4) = h^{-1}[g(3) - 4g(2)g(\frac{k}{h}) - 3(g(1))^2/h + 12g(1)g(\frac{k}{h})^2 - 6g(\frac{k}{h})^3].
\]
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],

\[
(8) \quad h(x) = \frac{e^{-x^2}}{x+1 - \frac{k}{2} \frac{(k-1)}{2} \frac{(k-2)}{2} \frac{2}{x+1}}.
\]

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,

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

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

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

For the initial estimate, \( x_0 \), we take, using the Hilferty-Wilson approximation (cf., Kendall and Stuart, [2], page 373)
\[ x_0 = k \left[ 2\left(\frac{1}{2} - \frac{1}{9k}\right) + z_p (\frac{2}{9k})^2 \right]^2, \]

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

\[ \alpha_n = 0 \]

\[ \gamma_n = -\frac{1}{6} \frac{f^{(3)}(x_n)}{f^{(2)}(x_n)} \]

\[ \beta_n = -\frac{1}{12} \frac{f^{(4)}(x_n)}{f^{(2)}(x_n)} + \frac{5}{36} \left[ \frac{f^{(3)}(x_n)}{f^{(2)}(x_n)} \right]^2, \]

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

With \( p \) and \( k \) specified, find \( z_p \) and \( x_0 \) using equation (10). Having determined \( x_{n-1}(n=1,2,\ldots) \), 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

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

Finally,

\[x_n = x_{n-1} + \frac{(t_{n-1} + \gamma_{n-1}t_{n-1}^2)}{(1 - \alpha_{n-1} - \beta_{n-1}t_{n-1}^2)}.\]

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 \((1-p)^{th}\) percentile for the chi-square distribution with \(k\) degrees of freedom is, to the prescribed degree of accuracy,

\[\chi^2_p(k) = 2y_p(k).\]

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

4. **Alternate Method for Computation of** \(\chi^2_p(k)\) (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 \(\chi^2_p(k)\) 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
\[
 f_T(t) = \frac{v^{-1/6}}{\Gamma(v+1/3)} e^{-v^{1/3} + \frac{1}{3} v t v^{-1/6}} (v^{1/3} + \frac{1}{3} t v^{-1/6})^3 v (0 < t < \infty),
\]
where, for convenience, the subscript, \( k \) on \( T_k \) has been suppressed.

Using the asymptotic expansion (cf. Whittaker and Watson, \( [4], \) page 252),
\[
 \log \Gamma(x) = (x - \frac{1}{2}) \log x - x + \frac{1}{2} \log(2\pi) + \frac{1}{12x} - \frac{1}{360x^3} + \cdots,
\]
we obtain
\[
 f_T(t) \sim \varphi(t) (1 + \frac{1}{36v} + \frac{17}{2592v^2} + \cdots) (1 - \frac{t^4}{108v} + \frac{t^5}{405v^{3/2}}
\]
\[
 + \frac{1}{v^2} \left[ \frac{t^8}{2328} - \frac{t^6}{1458} \right] + \frac{1}{v^{5/2}} \left[ \frac{t^7}{5103} - \frac{t^9}{43740} \right] + \cdots,
\]
where \( \varphi(t) = e^{-t^2/2\sqrt{2\pi}}. \) Thus
\[
\int_{\xi}^{\infty} f_T(t) dt \sim N_o(\xi) + \frac{1}{v^{3/2}} \left[ \frac{N_5(\xi)}{405} \right]
\]
\[
+ \frac{1}{v^2} \left[ \frac{17}{2592} - \frac{N_4(\xi)}{5888} - \frac{N_6(\xi)}{1458} + \frac{N_8(\xi)}{23328} \right]
\]
\[
+ \frac{1}{v^{5/2}} \left[ \frac{N_7(\xi)}{14580} + \frac{N_9(\xi)}{5103} - \frac{N_{10}(\xi)}{43740} \right] + \cdots,
\]

8
where

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

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

\[
\int_\xi^\infty f_T(t)dt = p + \sum_{n=2}^\infty v^{-n/2} G_n(z_p) + (N_0'(z_p) + \sum_{n=2}^\infty v^{-n/2} G_n(z_p)) (\xi-z_p) + \frac{1}{2} (N_0''(z_p) + \sum_{n=2}^\infty v^{-n/2} G_n''(z_p)) (\xi-z_p)^2 + \cdots.
\]

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

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

\[
c_4 = \phi^{-1}(z_p)[G_4(z_p)+c_2G_2(z_p) + \frac{1}{2} c_2^2 \phi(z_p) z_p],
\]

\[
c_5 = \phi^{-1}(z_p)[G_5(z_p)+c_3G_3(z_p)+c_2G_3(z_p)+c_2c_3G_2(z_p)+c_2^2 \phi(z_p)]
\]

Upon application of the relations, \(N_r(z) = \phi(z)z^{r-1} + (r-1)N_{r-2}(z)\) and
$N'_r(z) = -z^r \phi(z)$ $(r=1,2,\ldots)$, and simplification we obtain

$$c_2 = -\frac{1}{100} (z_p^3 + 3z_p) \quad c_3 = \frac{1}{405} (z_p^4 + 4z_p^2 + 8)$$

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

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

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

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

using equation (6) and since

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

Calculations, using the approximation,

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

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,

\[ D_n = \frac{e^{-x_k/2}}{x + \frac{1}{k/2^+}} \cdot \ldots \cdot \frac{[k/2-(n-1)](n-1)}{x + (2n-1) - k/2} \]

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

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</tr>
<tr>
<td>2</td>
<td>0.1105998097 (-15)</td>
</tr>
<tr>
<td>3</td>
<td>0.1105998181 (-15)</td>
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<td>4</td>
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<td>5</td>
<td>0.1105998186 (-15)</td>
</tr>
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<td>0.168902569 (-2)</td>
</tr>
<tr>
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<td>0.1661317266 (-2)</td>
</tr>
<tr>
<td>8</td>
<td>0.1661317313 (-2)</td>
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<tr>
<td>9</td>
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</tr>
<tr>
<td>18</td>
<td>0.1000132509</td>
</tr>
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</table>
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 $x = 46.4$.

\begin{align*}
  f(x) &= -4.83668 \ 06556 \ 61 \\
  f^{(1)}(x) &= -0.95782 \ 46788 \\
  f^{(2)}(x) &= -0.00088 \ 89830 \ 100 \\
  f^{(3)}(x) &= 0.0003 \ 74597 \ 5383 \\
  f^{(4)}(x) &= -0.00000 \ 23666 \ 47654 \\
  f(x_1) &= -0.08657 \ 06189 \ 89 \\
  f^{(1)}(x_1) &= -0.95288 \ 79229 \\
  f^{(2)}(x_1) &= -0.00110 \ 91574 \ 19 \\
  f^{(3)}(x_1) &= 0.00005 \ 21966 \ 2219 \\
  f^{(4)}(x_1) &= -0.00000 \ 36824 \ 80654 \\
  f(x_2) &= 6.1 \times 10^{-9} * \\
  \alpha_0 &= 0 \\
  \gamma_0 &= 0.00702 \ 29602 \ 0 \\
  \beta_0 &= 0.00002 \ 47601 \ 2325 \\
  t_0 &= -5.15496 \ 3915 \\
  x_1 &= 41.42839 \ 064 \\
  \alpha_1 &= 0 \\
  \gamma_1 &= 0.00784 \ 32843 \ 50 \\
  \beta_1 &= 0.00003 \ 09130 \ 1835 \\
  t_1 &= -0.09092 \ 02279 \\
  x_2 &= 41.33753 \ 504 \\
\end{align*}

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

$$x^2_p(6) \approx 82.67507008,$$

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


Calculations of Upper Tail Percentiles for the Chi-Square Distribution

Technical Report, December 1, 1964

Rubin, Herman and Zidek, James V.

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Technical Report No. 102

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14. KEY WORDS

Mathematical Models of Group Behavior
Group Problem-Solving
Individuals vs. Group Problem-Solving

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It is highly desirable that the abstract of classified reports be unclassified. Each paragraph of the abstract shall end with an indication of the military security classification of the information in the paragraph, represented as (TS), (S), (C), or (U).

There is no limitation on the length of the abstract. However, the suggested length is from 150 to 225 words.

14. KEY WORDS: Key words are technically meaningful terms or short phrases that characterize a report and may be used as index entries for cataloging the report. Key words must be selected so that no security classification is required. Identifiers, such as equipment model designation, trade name, military project code name, geographic location, may be used as key words but will be followed by an indication of technical context. The assignment of links, rules, and weights is optional.