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An efficient algorithm for computing quantiles of the noncentral chi-squared distribution

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Abstract

An efficient algorithm is provided for computing quantiles of the noncentral chi-squared distribution. Newton's method, which requires the evaluations of both of the noncentral chi-squared distribution function and the density, is used. A close relationship between their recursive computing formulas is noted to allow concurrent evaluation of the distribution function and the density. Newton's iterative computation can therefore be greatly speeded up. An example is given to illustrate the usefulness of the algorithm. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

Let $F(x;r,\theta)$ and $f(x;r,\theta)$ denote, respectively, the noncentral chi-squared distribution function and the density with r (>0) degrees of freedom and noncentrality parameter θ (≥ 0), and $F(x;r)$ and $f(x;r)$ the central chi-squared distribution function and the density with r (>0) degrees of freedom. It is well known that (see, e.g., Johnson and Kotz, 1970b, p. 132)

$$F(x;r,\theta)=\sum_{i=0}^{\infty}(\lambda^i e^{-\lambda}/i!)F(x;r+2i), \tag{1}$$

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and

$$f(x;r,\theta)=\sum_{i=0}^{\infty}(\lambda^i e^{-\lambda}/i!)f(x;r+2i), \tag{2}$$

where $\lambda=\theta/2$. Let $x_{p;r,\theta}$ denote the p-quantile for which $F(x_{p;r,\theta};r,\theta)=p$ for $0<p<1$. To obtain $x_{p;r,\theta}$, one can apply any standard numerical root-finding method (see, e.g., Kennedy and Gentle, 1980, p. 72). A well-known efficient method is Newton's method, which requires the evaluations of $F(x;r,\theta)$ and its derivative $f(x;r,\theta)$. Johnson and Pearson (1969) used Newton's method to compute $x_{p;r,\theta}$ and prepared tables for $\sqrt{x_{p;r,\theta}}$. However, as mentioned in Boomsma and Molenaar (1994), no specific algorithm for computing $x_{p;r,\theta}$ is readily available in the literature. In this article, we revisit Newton's method by discovering a close relationship between recursive formulas for evaluating $F(x;r,\theta)$ and $f(x;r,\theta)$ in such a way that $F(x;r,\theta)$ and $f(x;r,\theta)$ can be evaluated concurrently. Newton's iterative computation can therefore be greatly speeded up. The idea of concurrent evaluation in Newton's iterations to enhance computational efficiency was first seen in Ding (1994a) for computing noncentral beta quantiles. This important idea was also applied in later relevant work (Ding, 1994b,1996,1997; Tiwari and Yang, 1997). The article is organized as follows. In Section 2, numerical treatments for computing $x_{p;r,\theta}$ are discussed. The discussions include how to deal with extreme value cases. The resulting efficient algorithm is specifically presented in Section 3. In Section 4, an example demonstrating sample size determination in a simple situation of interval testing is given to illustrate the usefulness of the algorithm.

2. Numerical methods

To compute $x_{p;r,\theta}$ using Newton's method, repeat the iteration

$$x_{j+1}=x_j-\frac{F(x_j;r,\theta)-p}{f(x_j;r,\theta)},\quad j=0,1,2,\ldots \tag{3}$$

until $|x_{j+1}-x_j|\le\delta x_{j+1}$, where δ denotes a convergence criterion. Both $F(x;r,\theta)$ and $f(x;r,\theta)$ need to be evaluated at each iteration. Farebrother (1987) developed a recursive algorithm to evaluate (1) for integer degrees of freedom and proposed an upper bound on the error of truncating the series to control the computational accuracy. Posten (1989) provided a more complete algorithm in a step-by-step form for real degrees of freedom. The algorithm basically reduces the problem to that of evaluating a single central chi-squared distribution function. Ding (1992) gave a computationally simple algorithm based on an alternative series representation. In fact, due to the properties that (see, e.g., Ding, 1992; Posten, 1989)

$$F(x;r)=2f(x;r+2)+F(x;r+2), \tag{4}$$

and

$$f(x;r+2i)=\frac{x}{r+2i-2}f(x;r+2i-2),\quad i=1,2,\ldots \tag{5}$$

the recursive formulas for computing $F(x;r,\theta)$ and $f(x;r,\theta)$ are closely related as follows:

$$F(x;r,\theta)=\sum_{i=0}^{\infty}P(i)W(i), \tag{6}$$

$$f(x;r,\theta)=\sum_{i=0}^{\infty}P(i)D(i), \tag{7}$$

where $P(i)=\lambda^i e^{-\lambda}/i!$, $W(i)=F(x;r+2i)$, $D(i)=f(x;r+2i)$, and

$$\begin{aligned}&P(0)=e^{-\lambda},\quad W(0)=F(x;r),\quad D(0)=f(x;r)=\frac{1}{\Gamma(r/2)2^{r/2}}x^{r/2-1}e^{-x/2},\\&P(i)=(\lambda/i)P(i-1),\quad D(i)=\frac{x}{r+2i-2}D(i-1),\\&W(i)=W(i-1)-2D(i),\quad i=1,2,\ldots\end{aligned} \tag{8}$$

It follows that evaluations of $F(x;r,\theta)$ and $f(x;r,\theta)$ should be combined for each iteration in Eq. (3) to enhance the computational efficiency of Newton's method. In the recursive evaluation of Eqs. (6) and (7) through Eq. (8), $F(x;r)$ is the only central chi-squared distribution function that needs to be evaluated.

For extremely large values of noncentrality parameter, the summations of the series in Eqs. (6) and (7) should be started at a higher index to avoid floating point underflow. By following the remark given by Frick (1990), we have

$$\sum_{i=0}^{m-1}P(i)W(i)\le\sum_{i=0}^{m-1}P(i)W(0)<\sum_{i=0}^{m-1}P(i)\le\Phi((m-\lambda)/\sqrt{\lambda}),$$

and

$$\sum_{i=0}^{m-1}P(i)D(i)\le\sum_{i=0}^{m-1}P(i)\le\Phi((m-\lambda)/\sqrt{\lambda}), \tag{9}$$

where Φ denotes the standard normal distribution function. It appears that the errors in omitting the first m terms of two series, referred to as the lower truncation errors, are both bounded above by $\Phi((m-\lambda)/\sqrt{\lambda})$. For a specified error bound ε, the starting index m is determined by $m=[\max(\lambda+U_\varepsilon\sqrt{\lambda},0)]$, where U_ε is the ε-quantile of the standard normal distribution, and $[\cdot]$ denotes 'largest integer less than or equal to'.

In contrast to the lower truncation error, $\sum_{i=n}^{\infty}P(i)W(i)$ is the error of truncating the series in Eq. (6) at $i=n$ $(n>m)$, and is referred to as the upper truncation error. It is bounded above by $b_F(n)=[1-\sum_{i=m}^{n-1}P(i)]W(n)$ since (see also Farebrother, 1987)

$$\sum_{i=n}^{\infty}P(i)W(i)<\sum_{i=n}^{\infty}P(i)W(n)=\left[1-\sum_{i=0}^{n-1}P(i)\right]W(n)\le\left[1-\sum_{i=m}^{n-1}P(i)\right]W(n). \tag{10}$$

On the other hand, the upper truncation error $\sum_{i=n}^{\infty} P(i)D(i)$ $(n>m)$ of the series in Eq. (7) is bounded above by $b_f(n)=[1-\sum_{i=m}^{n-1} P(i)]D(n)$ under the condition that $r+2n>x$, since, under this condition, the sequence $\{D(i)\}$ $(i \geq n)$ is decreasing, and therefore

$$\sum_{i=n}^{\infty} P(i)D(i) < \sum_{i=n}^{\infty} P(i)D(n) = \left[1-\sum_{i=0}^{n-1} P(i)\right] D(n) \leq \left[1-\sum_{i=m}^{n-1} P(i)\right] D(n). \tag{11}$$

Note that $b_F(n)$ decreases as n increases; so does $b_f(n)$ when $r+2n>x$. The upper truncation errors can be controlled by using $b_F(n)$ and $b_f(n)$, which are easy to compute because they rely only on factors that are computed in the course of evaluating Eqs. (6) and (7).

Given a bound ε on the lower truncation errors and another bound ε' on the upper truncation errors, the series in Eqs. (6) and (7) are approximated by the finite sums $\sum_{i=m}^{n_1} P(i)\,W(i)$ and $\sum_{i=m}^{n_2} P(i)\,D(i)$, respectively, where $m=[\max(\lambda + U_\varepsilon\sqrt{\lambda}, 0)]$, $n_1(\geq m)$ is the minimum integer satisfying $b_F(n_1) \leq \varepsilon'$, and n_2 $(\geq m)$ is the minimum integer satisfying $r+2n_2>x$ and $b_f(n_2) \leq \varepsilon'$. The terms are computed recursively by Eq. (8) with the starting factors $P(m)=\lambda^m e^{-\lambda}/m!$, $W(m)=F(x;r+2m)$, and $D(m)=f(x;r+2m)=x^{r/2+m-1}e^{-x/2}/(\Gamma(r/2+m)2^{r/2+m})$. The approximations to the series have an error bound of $\varepsilon+\varepsilon'$. Due to the close relationship between their computing formulas, $F(x;r,\theta)$ and $f(x;r,\theta)$ are evaluated concurrently rather than independently within each Newton's iteration in Eq. (3). Redundant computations can therefore be avoided, and the computational efficiency of Newton's method enhanced.

A starting value x_0 for Newton's iteration (3) should be well determined. Extensive tests show that, when p is not very small, $x_{p;r,\theta}$ can be well approximated by using the Cornish–Fisher expansion (see, e.g., Johnson and Kotz, 1970a, p. 34) with the first four terms. The approximation requires the evaluations of U_p and the first four cumulants, $k_1=r+\theta$, $k_2=2(r+2\theta)$, $k_3=8(r+3\theta)$, and $k_4=48(r+4\theta)$ of $F(x;r,\theta)$. It is given by

$$x_{p;r,\theta} \approx k_1 + k_2^{1/2}[U_p + \gamma_1(U_p^2-1)/6 + \gamma_2(U_p^3-3U_p)/24 - \gamma_1^2(2U_p^3-5U_p)/36], \tag{12}$$

where $\gamma_1=k_3/k_2^{3/2}$, and $\gamma_2=k_4/k_2^2$. Using the approximation (12) to be x_0 would lead to fast convergence for most cases. For small values of p, the starting value x_0 and iterates x_{j+1} may be nonpositive. If $x_0 \leq 0$, then replace it by δ. In subsequent iterations, if $x_{j+1} \leq 0$, set $x_{j+1}=x_j/10$. Note that the number of iterations needs to be controlled.

3. The algorithm

Based on the discussions given in Section 2, an efficient algorithm, named NCX2Q, is developed for computing quantiles $x_{p;r,\theta}$ of the noncentral chi-squared distribution.

Three auxiliary algorithms for evaluating U_ε (e.g., Beasley and Springer, 1977), the natural logarithm of the gamma function (e.g., Macleod, 1989; Pike and Hill, 1966), and the central chi-squared distribution function (e.g., Lau, 1980; Posten, 1989; Shea, 1988) are required.

Algorithm NCX2Q

Step 1: Input $r =$ degrees of freedom, $\theta =$ noncentrality parameter, and $p =$ cumulative probability ($0 < p < 1$). Specify and input $\varepsilon =$ the desired error bound for evaluating $F(x; r, \theta)$ and $f(x; r, \theta)$, $\delta =$ convergence criterion for Newton's iterative process, and $M_{\max} =$ the maximum number of Newton's iterations allowed.

Step 2: Evaluate $\lambda = \theta/2$. If $\lambda = 0$, then $m = 0$, and $P(m) = 1$; otherwise $m = [\max(\lambda + U_{\varepsilon/2}\sqrt{\lambda}, 0)]$, and $P(m) = \exp[m \ln \lambda - \lambda - \ln \Gamma(m+1)]$. Evaluate $\mathrm{CONST} = \ln \Gamma(r/2 + m) + (r/2 + m) \ln 2$.

Step 3: Evaluate x_0 (by Formula (12)). If $x_0 \le 0$, then $x_0 = \delta$.

Step 4: For $j = 0, 1, \ldots, M_{\max} - 1$, do Steps 4.1 through 4.5.

Step 4.1: Evaluate $W(m) = F(x_j; r + 2m)$, $D(m) = \exp[(r/2 + m - 1) \ln x_j - x_j/2 - \mathrm{CONST}]$, $\mathrm{PSUM} = P(m)$, $\mathrm{CDF} = P(m)W(m)$, and $\mathrm{PDF} = P(m)D(m)$.

Step 4.2: For $i = m+1, m+2, \ldots,$ (halt when accumulations of PDF and CDF are both stopped)

evaluate

$P(i) = (\lambda/i)P(i-1)$,

$D(i) = D(i-1)x_j/(r + 2i - 2)$,

$\mathrm{PDF} = \mathrm{PDF} + P(i)D(i)$, (stop accumulation when $r + 2i > x_j$ and $(1 - \mathrm{PSUM})D(i) \le \varepsilon/2$)

$W(i) = W(i-1) - 2D(i)$,

$\mathrm{CDF} = \mathrm{CDF} + P(i)W(i)$, (stop accumulation when $(1 - \mathrm{PSUM})W(i) \le \varepsilon/2$)

and

$\mathrm{PSUM} = \mathrm{PSUM} + P(i)$.

Step 4.3: Evaluate $\mathrm{DIFF} = (\mathrm{CDF} - p)/\mathrm{PDF}$.

Step 4.4: If $x_j - \mathrm{DIFF} \le 0$, then $x_{j+1} = x_j/10$; otherwise $x_{j+1} = x_j - \mathrm{DIFF}$.

Step 4.5: If $|\mathrm{DIFF}| \le \delta x_{j+1}$, then Output $x_{p;r,\theta} = x_{j+1}$.

Step 5: Output the error message, 'No convergence after $M_{\max}$ iterations'.

4. An application of the algorithm

To illustrate the usefulness of the proposed algorithm, this section discusses how to determine the sample size required in a simple situation of interval testing. Let $X_1, X_2, \ldots, X_N$ denote a random sample of size N from a normal distribution with mean μ (unknown) and variance σ_0^2 (known). Without loss of generality, set $\sigma_0^2 = 1$. Suppose that we are interested in testing the hypothesis $\mathrm{H}_0: |\mu - \mu_0| \le \tau_0$ ($\tau_0 > 0$) against H_1: $|\mu - \mu_0| > \tau_0$. A UMP unbiased test with level of significance α is given

Table 1
The minimum sample size required ($\hat{N}$) for selected combinations of τ_0, τ_1, α and p^*

τ_0	τ_1	α	p^*	$\hat{N}$
0.01	0.05	0.10	0.90	4193
			0.95	5412
	0.10	0.10	0.90	900
			0.95	1144
0.1	0.3	0.01	0.95	395
			0.99	542
	0.6	0.01	0.95	64
			0.99	87
	0.9	0.01	0.95	25
			0.99	34
0.2	0.6	0.05	0.95	68
			0.99	99
	1.2	0.05	0.95	11
			0.99	16
	1.8	0.05	0.95	5
			0.99	7

by (see, e.g., Lehmann, 1986, p. 135)

$$\phi(\boldsymbol{x}) = \begin{cases} 1 & \text{if } |\sqrt{N}(\bar{x} - \mu_0)| \geq c', \\ 0 & \text{otherwise,} \end{cases}$$

where c' is chosen so that $P(|\sqrt{N}(\bar{X} - \mu_0)| \geq c' \mid \mu = \mu_0 \pm \tau_0) = \alpha$, or equivalently,

$$\phi(\boldsymbol{x}) = \begin{cases} 1 & \text{if } N(\bar{x} - \mu_0)^2 \geq (c')^2 = c, \\ 0 & \text{otherwise,} \end{cases}$$

where c is chosen so that $P(N(\bar{X} - \mu_0)^2 \geq c \mid \mu = \mu_0 \pm \tau_0) = \alpha$. Since the test statistic, $N(\bar{X} - \mu_0)^2$, has a noncentral chi-squared distribution with one degree of freedom and noncentrality parameter $\theta = N(\mu - \mu_0)^2$, the critical value c can be obtained by invoking Algorithm $NCX2Q$ with $p = 1 - \alpha, r = 1$, and $\theta = N\tau_0^2$. An interesting problem in the above interval testing is sample size determination based on a given power. For a specified value μ_1 of μ under H_1, we have $\tau_1 = |\mu_1 - \mu_0| > \tau_0$, and $\theta = N\tau_1^2$. It is desired to find the minimum sample size required, denoted by $\hat{N}$, to achieve a specified power p^* $(> \alpha)$ at the alternative, i.e., to find $\hat{N}$ such that $1 - F(x_{1-\alpha;1,\hat{N}\tau_0^2}; 1, \hat{N}\tau_1^2) \geq p^*$. A simple iterative procedure given below may be used:

Step 1: Input τ_0, τ_1 $(> \tau_0), \alpha$, and p^* $(> \alpha)$.
Step 2: For $N = 1, 2, \ldots,$
evaluate
$\theta_0 = N\tau_0^2$,
$\theta_1 = N\tau_1^2$,
$c = x_{1-\alpha;1,\theta_0}$, (by invoking $NCX2Q$)

and

$$p' = 1 - F(c; 1, \theta_1)$$

until $p' \geq p^*$.

Step 3: Output $\hat{N} = N$.

Algorithm *NCX2Q* and another algorithm for evaluating the noncentral chi-squared distribution function (e.g., Posten, 1989) are needed in the procedure. Table 1 shows the values of $\hat{N}$ obtained for selected combinations of τ_0, τ_1, α and p^*. It appears that the efficiency of computing quantiles of the noncentral chi-squared distribution is important in this application, especially when τ_1 is close to τ_0.

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