A NOTE ON BOUNDS FOR THE ASYMPTOTIC SAMPLING VARIANCE OF THE MAXIMUM LIKELIHOOD ESTIMATOR OF A PARAMETER IN THE NEGATIVE BINOMIAL DISTRIBUTION

BY L. R. SHENTON (Received May 13, 1963)

1. Introduction

Using the notation

(1)
$$P_{z} = \frac{\alpha(\alpha+1)\cdots(\alpha+\chi-1)}{\chi!} \frac{\lambda^{z}\alpha^{\alpha}}{(\lambda+\alpha)^{\alpha+\chi}}$$
$$(\alpha, \lambda > 0; \chi = 0, 1, \cdots)$$

for the probability function of a negative binomial variate, the asymptotic variance of the maximum likelihood estimate $\hat{\alpha}$ of α is

(2)
$$(n \operatorname{Var} \widehat{\alpha})^{-1} = k \sum_{s=2}^{\infty} u_s = k U(\lambda, \alpha)$$

where

$$\begin{split} k &= \frac{1}{2} \left(\frac{\lambda}{\lambda + \alpha} \right)^2 \frac{1}{\alpha(\alpha + 1)} , \\ u_s &= \frac{2}{s} \left(\frac{\lambda}{\lambda + \alpha} \right)^{s-2} \frac{(s-1)!}{(\alpha + s - 1)^{(s-2)}} . \end{split}$$

A series implying (2) was given by Fisher (1941) who derived it by transforming the series for i_{kk} , namely

(3)
$$i_{kk} = \left(\frac{\alpha}{\lambda + \alpha}\right)^{\alpha} \sum_{s=1}^{\infty} \frac{(\alpha + s - 1)!}{(\alpha - 1)! \, s!} \left(\frac{\lambda}{\lambda + \alpha}\right)^{s} \sum_{t=0}^{s-1} \frac{1}{(\alpha + t)^{2}}.$$

In a recent paper Shenton and Wallington ([3], expressions (21b) and (21d)) have given approximations to U when λ/α is large and when α is not small. In passing we remark that they fail to point out that one of their expressions is tantamount to

(4)
$$(n \operatorname{Var} \hat{\alpha})^{-1} \sim \Psi^{(1)}(\alpha) - 1/\alpha (\lambda \operatorname{large})$$

where $\Psi^{(1)}(\alpha) = D_{\alpha}^2 \log \Gamma(\alpha)$ and is the *trigamma* function.

2. Elementary bounds

Since the sampling variance of $\hat{\alpha}$ has not been tabulated to any extent it seems desirable to find useful bounds and approximations. From (2)

$$U(\lambda, \alpha) = 1 + \frac{2 \cdot 2!}{3(\alpha+2)} \frac{\lambda}{\lambda+\alpha} + \frac{2 \cdot 3!}{4(\alpha+2)(\alpha+3)} \left(\frac{\lambda}{\lambda+\alpha}\right)^2 + \cdots$$

so that for $\alpha > 0$, $\lambda \ge 0$,

$$U(\lambda, \alpha) \ge 1$$

and

$$U(\lambda, \alpha) \leq 1 + \frac{2 \cdot 2!}{3(\alpha + 2)} + \frac{2 \cdot 3!}{4(\alpha + 2)(\alpha + 3)} + \cdots$$
$$= 2\alpha(\alpha + 1)(\Psi^{(1)}(\alpha) - 1/\alpha).$$

We deduce that

$$(5) \qquad (1+\alpha/\lambda)^2/(\Psi^{(1)}(\alpha)-1/\alpha) < n \operatorname{Var} \widehat{\alpha} < 2\alpha(\alpha+1)(1+\alpha/\lambda)^2,$$

and the lower bound may be evaluated by referring to tables of $\Psi^{(1)}(\alpha)$ (for example, H. T. Davis, Tables of Higher Mathematical Functions, Principia Press, Bloomington). If we use the mean of the two bounds in (5), then the relative error of this approximation is at most

(6)
$$e(\alpha) = \alpha(\alpha+1)(\Psi^{(1)}(\alpha)-1/\alpha)-1/2$$

$$= \alpha(\alpha+1)\left\{\frac{1}{2\alpha^{2}} + \frac{B_{2}}{\alpha^{3}} - \frac{B_{4}}{\alpha^{5}} - \frac{B_{5}}{\alpha^{7}} - \cdots\right\} - \frac{1}{2} \quad (\alpha \text{ large})$$

where $B_2=1/6$, $B_4=-1/30$, $B_6=1/42$, etc. are Bernoulli numbers, so that $e(\alpha)$ is about 7 per cent or less if α exceeds 10 and about 15 per cent or less if $5<\alpha<10$. However, the error may be considerable if α is small.

3. Integral representation

It is readily verified that

(17)
$$U(\lambda, \alpha) = \frac{2\alpha(\alpha+1)}{\theta} \{V(\theta, \alpha) - 1/\alpha\}$$

(8) where
$$\theta V(\theta, \alpha) = -\int_0^1 \frac{t^{\alpha-1} \log \{1 - \theta(1-t)\} dt}{1-t}$$
 $(\alpha > 0, 0 < \theta < 1)$

and $\theta = \lambda/(\lambda + \alpha)$. Now taking α and θ as independent variables we have

(9a)
$$\theta\{V(\theta, \alpha) - V(\theta, \alpha+1)\} = \frac{\theta}{\alpha} \int_0^1 \frac{(1-t)^{\alpha}dt}{1-\theta t}$$

$$= \frac{1}{\alpha} \int_0^1 \frac{t^{\alpha}}{z+t} dt \quad \left(z = \frac{1-\theta}{\theta}\right).$$

We deduce from (9) the expansions in terms of hypergeometric functions

(10a)
$$V(\theta, \alpha) = \sum_{s=1}^{\infty} \frac{F(1, 1; \alpha+s+1; \theta)}{(\alpha+s-1)(\alpha+s)} \quad (\alpha > 0, 0 < \theta < 1),$$

(10b)
$$= \frac{1}{1-\theta} \sum_{s=1}^{\infty} \frac{F(1, \alpha+s; \alpha+s+1; -\theta/(1-\theta))}{(\alpha+s-1)(\alpha+s)} \quad (\alpha > 0, \ 0 < \theta < \frac{1}{2}).$$

Actually (10a) is equivalent to a generalization of (4), for if λ is large, we use Gauss's theorem

$$F(a, b; c; 1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} \quad (c>a+b)$$

and derive

$$V(\theta, \alpha) \sim \sum_{s=1}^{\infty} \frac{1}{(\alpha+s-1)^2}$$
 (λ large).

Comparing (10a) with the behaviour of the derivative of the Psi function when the argument is small leads one to expect relatively slow convergence in this case.

4. Continued fraction bounds

From (9b) we have

(11)
$$\theta V(\theta, \alpha) = \int_0^1 \frac{t^{\alpha} f(t)}{z+t} dt \sim \frac{\mu_0}{z} - \frac{\mu_1}{z^2} + \frac{\mu_2}{z^3} - \cdots$$

where

$$f(t) = \sum_{s=0}^{\infty} \frac{t^s}{\alpha + s}, \ \mu_s = \frac{1}{s+1} \sum_{r=0}^{s} \frac{1}{\alpha + r}$$

and in fact (11) can be written in the form of a Stieltjes transform

(12)
$$\alpha\theta V(\theta, \alpha) = \int_0^\infty \frac{dF(t)}{z+t},$$

where the distribution function F(t), with moments $\alpha \mu_i$, is defined as

(13)
$$F(t) = \alpha \int_{0}^{t} \frac{(t-u)u^{\alpha-1}du}{1-u} \quad 0 \le t \le 1;$$

$$F(t) = 1, \quad t > 1$$

$$F(t) = 0, \quad t < 0.$$

Evidently F(t) is bounded and non-decreasing and has infinitely many different values for t>0. Moreover, it may be verified that

(14)
$$\sum_{0}^{\infty} (1/\mu_{s})^{(1/2s)} = \infty.$$

Hence the Stieltjes moment problem is determinate (see for example Wall [5], or Shohat and Tamarkin [4]), and there is the Stieltjes continued fraction development

(15)
$$\alpha\theta V(\theta, \alpha) = \frac{1}{z+} \frac{p_1}{1+} \frac{q_1}{z+} \frac{p_2}{1+} \frac{q_2}{z+} \cdots,$$

where the p's and q's are positive (and actually functions of α only) and evaluated from

$$p_n = \frac{A_{n-1}B_n}{A_nB_{n-1}}$$
, $q_n = \frac{A_{n+1}B_{n-1}}{A_nB_n}$, $(A_0 = B_0 = 1)$

with

$$A_n = egin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} \ \mu_1 & \mu_2 & \cdots & \mu_n \ & \ddots & & \ddots & & \ & \mu_{n-1} & \mu_n & \cdots & \mu_{2n-2} \end{bmatrix} \quad B_n = egin{bmatrix} \mu_1 & \mu_2 & \cdots & \mu_n \ \mu_2 & \mu_3 & \cdots & \mu_{n+1} \ & \ddots & & \ddots & & \ & \mu_n & \mu_{n+1} & \cdots & \mu_{2n-1} \end{bmatrix} \quad (n=1,\,2,\,\cdots) \, .$$

The continued fraction expansion (15) converges for $\alpha>0$ and $\lambda\geq0$ but the p's and q's soon become complicated; however it can be shown that they never exceed unity (this follows from the fact that the moment problem for the interval (0,1) is determinate) and moreover, using a theorem of Chokhatte [1]

$$\lim_{n\to\infty} p_n = \lim_{n\to\infty} q_n = 1/4.$$

It is conjectured that p_n monotonically decreases to a quarter and that q_n monotonically increases to a quarter.

It may be pointed out that if the p's and q's are evaluated for a particular value of α then V can be evaluated for different λ merely by changing z in (15).

Again the odd and even convergents in (15) give upper and lower bounds respectively of increasing accuracy to V, and hence lower and upper bounds of increasing accuracy to n Var $\hat{\alpha}$.

The first few partial numerators in the continued fraction are:

$$p_{i} = \frac{2\alpha + 1}{2\alpha + 2} \qquad q_{i} = \frac{5\alpha + 2}{6(\alpha + 1)(\alpha + 2)(2\alpha + 1)}$$

$$p_{i} = \frac{(\alpha + 1)R}{3(\alpha + 2)(\alpha + 3)(2\alpha + 1)(5\alpha + 2)} \qquad q_{i} = \frac{4(2\alpha + 1)S}{5(\alpha + 3)(\alpha + 4)(5\alpha + 2)R}$$

$$p_{i} = \frac{3(\alpha + 2)(5\alpha + 2)T}{10(\alpha + 4)(\alpha + 5)RS} \qquad q_{i} = \frac{27RU}{14(\alpha + 5)(\alpha + 6)ST}$$

where

$$R = 30\alpha^{3} + 78\alpha^{3} + 58\alpha + 12,$$

$$S = 245\alpha^{3} + 587\alpha^{2} + 390\alpha + 72$$

$$T = 4,900\alpha^{6} + 36,070\alpha^{5} + 102,608\alpha^{4} + 143,084\alpha^{3} + 101,958\alpha^{3} + 34,704\alpha + 4,320$$

$$U = 140,161\alpha^{6} + 990,172\alpha^{5} + 2,683,877\alpha^{4} + 3,536,882\alpha^{3} + 2,360,376\alpha^{2} + 747,360\alpha + 86,400.$$

As examples of the bounds we have

(16)
$$\alpha^2(\lambda+\alpha)/\lambda^2 < n \operatorname{Var} \hat{\alpha} < \alpha(\lambda+\alpha) \{(2\alpha+1)\lambda+2\alpha^2+2\alpha\}/\lambda^2$$
 and somewhat closer

(17)
$$2\alpha^{2}(\alpha+1)(\lambda+\alpha)V/\lambda^{2} < n \operatorname{Var} \widehat{\alpha} < 2\alpha(\alpha+1)(\lambda+\alpha)W/\lambda^{2}$$

where

$$V = \frac{(6\alpha^{2} + 12\alpha + 4)\lambda + 3\alpha(\alpha + 2)(2\alpha + 1)}{(5\alpha + 2)\lambda + 3\alpha(\alpha + 2)(2\alpha + 1)},$$

$$W = \frac{(2\alpha + 1)a_{1}\lambda^{2} + 3\alpha(\alpha + 2)a_{2}\lambda + 3\alpha^{2}(\alpha + 2)(\alpha + 3)(2\alpha + 1)(5\alpha + 2)}{a_{3}\lambda + 3\alpha(\alpha + 2)(\alpha + 3)(2\alpha + 1)(5\alpha + 2)}$$

with

$$\begin{cases} a_1 = 15\alpha^3 + 39\alpha^3 + 29\alpha + 6 \\ a_2 = 20\alpha^3 + 50\alpha^2 + 32\alpha + 6 \\ a_3 = 30\alpha^4 + 133\alpha^3 + 231\alpha^2 + 134\alpha + 24 \end{cases}.$$

5. Bounds depending on the trigamma function

It is easily shown that

(18)
$$\frac{1}{n \operatorname{Var} \hat{\alpha}} = \Psi^{(1)}(\alpha) - \frac{\lambda}{\alpha(\lambda + \alpha)} - \frac{\Phi}{\lambda} \qquad (\alpha, \lambda, >0)$$

where

$$\Phi = \int_0^\infty \frac{dF(t)}{t(t+z)}.$$

A sequence of increasing lower bounds can now be set up using a result on generalized continued fractions given by Shenton ([2], (48)). It turns out that

(19)
$$\Phi = \lim_{s \to \infty} \rho_s$$

where $\rho_s = k_s^*/k_s$, and k_s^* , k_s follow the recurrence

$$\left\{ \begin{array}{l} u_{2s} = u_{2s-1} + \alpha_{2s} u_{2s-2} - \beta_{2s} u_{2s-4} - \gamma_{2s} u_{2s-5} + \delta_{2s} u_{2s-6} \\ u_{2s-1} = \alpha_{2s-1} u_{2s-3} - \beta_{2s-1} u_{2s-5} + \delta_{2s-1} u_{2s-7} \end{array} \right.$$
 (s=2, 3, \cdots)

with

$$k_0^*=0$$
, $k_1^*=k_2^*=1$; $k_s^*=0$, $s<0$; $k_0=1$, $k_1=0$, $k_2=b_3(z+b_2+b_3)$; $k_s=0$, $s<0$;

and

$$\alpha_s = b_s(z + b_{s-1} + b_s + b_{s+1}), \ \beta_s = b_{s-2}b_s\alpha_{s-1},$$
 $\gamma_s = b_{s-3}b_{s-2}b_{s-2}b_{s-1}b_s, \ \delta_s = b_{s-4}b_{s-3}b_{s-2}^2b_{s-1}b_s;$

where $b_{2s}=p_s$, $b_{2s+1}=q_s$ and are given in terms of the partial numerators of (15).

Moreover.

$$\rho_2 < \rho_4 < \rho_5 < \cdots < \Phi$$
.

Using ρ_2 we find

(20)
$$n \operatorname{Var} \widehat{\alpha} > \left[\Psi^{(1)}(\alpha) - \frac{\lambda}{\alpha(\lambda + \alpha)} - \frac{6(\alpha + 1)(\alpha + 2)}{2\lambda(3\alpha^2 + 6\alpha + 2) + 3\alpha(\alpha + 2)(2\alpha + 1)} \right]^{-1}$$
.

6. Concluding remarks

A number of assessments are given for the large sample variance of the maximum likelihood estimate $\hat{\alpha}$ of α in the negative binomial dis-

tribution. The series (2) can be used to give upper bounds, and these are readily calculated from the partial sums provided α is not small and λ large—in which case the series converges slowly. If, however, λ/α is large, then bounds from the Stieltjes continued fraction (15) should be useful. Again if λ is large, then lower bounds can be calculated from (19).

VIRGINIA POLYTECHNIC INSTITUTE, U.S.A.

REFERENCES

- [1] J. Chokhatte, "Sur le développement de l'lintegrale $\int_a^b \frac{p(y)dy}{x-y}$ en fraction continue et sur les polynomes de Tchebycheff," Rendiconti Circole Matematico Palermo, T. 47 (1923), pp. 25-46.
- [2] L. R. Shenton, "A determinantal expansion for a class of definite integral. Proc. Edinburgh Math. Soc., Vol. 10 (1957), pp. 167-188.
- [3] L. R. Shenton and P. A. Wallington, "The bias of moment estimators with an application to the negative binomial distribution," *Biometrika*, Vol. 49 (1962), pp. 193-204.
- [4] J. A. Shohat and J. D. Tamarkin, The problem of moments, New York: American Math. Soc., (1943).
- [5] H. S. Wall, Analytic Theory of Continued Fractions. Van Nostrand, New York, (1948).