

MINIMUM VARIANCE ESTIMATION OF PROBABILITIES

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Abstract

This paper reviews the problem of estimating probabilities when complete sufficient statistics exist, and then discusses the problem of obtaining the variances of such estimators. In particular (Cramer-Rao) lower bounds and upper bounds for the variances are obtained.

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## 1. Introduction

Since the fundamental papers of Lehmann and Scheffé (6) much work has been done on finding explicit minimum variance unbiased estimators. The problem of unbiased estimation of distribution functions (or probability mass functions if the distribution is discrete) has, in particular, received attention by Tate (8), Barton (1).

The problem, simply stated is:

Given a random sample  $X_1, X_2, \dots, X_n$  from  $F_\theta$  find the uniformly minimum variance unbiased estimator of  $F_\theta(x_0) = P_\theta[X \leq x_0]$  or  $P_\theta[X = x_0]$  if  $F_\theta$  is discrete.

The problem in the generality stated above is much too difficult to admit a closed solution. When a complete sufficient statistic for  $\theta$  exists, however, it is usually possible to obtain explicit representations for the estimator of  $F_\theta(x_0)$  or  $P_\theta[X = x_0]$ . Such expressions for the hypergeometric, binomial, Poisson, exponential and normal distributions have been obtained by various authors e.g. Tate, Barton. What has not been done, however, is any calculations on the variance (known to be minimal) of these estimators or calculations leading to confidence intervals. The reason for this lack of calculation will become apparent when some of the expressions for the estimators are exhibited - in general the integrals (or sums) which must be evaluated are complicated. In this paper we present some of the estimators derived by previous workers and indicate the Cramer-Rao lower bound for their variance as well as a (crude) upper bound to their variance.

## 2. The estimators

Let  $X_1, X_2, \dots, X_n$  be independent with common distribution  $F_\theta$ . Recall that  $t(\underline{x})$  is sufficient for  $\theta$  if the conditional distribution of  $\underline{X}$  given  $t(\underline{x})$  is independent (functionally) of  $\theta$ . For computational purposes it is usual to demonstrate sufficiency by using the Fisher-Neyman factorization theorem which states that  $s(\underline{x})$  is sufficient for  $\theta$  if and only if we can write

$$f_\theta(\underline{x}) = h(\underline{x})g_\theta(s(\underline{x}))$$

where  $f_\theta(\underline{x})$  is the density or probability mass function of the sample. Also recall that the distribution of  $s(\underline{x})$  is said to be complete if it has the property that

$$\underline{e}_{\theta}[\underline{o}(s(\underline{x}))] = 0$$

for all  $\underline{\theta}$  implies that  $\underline{o}(s(\underline{x}))$  is the null function (with probability one).

Note that it is not necessary to find the distribution of  $s(\underline{x})$  to show completeness although it is sometimes convenient to do so.

If  $X_1, X_2, \dots, X_n$  are independent with common distribution  $F_{\theta}$  and a sufficient statistic  $s(\underline{x})$  exists whose distribution is complete the estimation of a parametric function  $\gamma(\underline{\theta})$  by means of minimum variance unbiased estimators has a rather satisfactory theory. The main result is

Theorem 1. Under the assumptions that  $s(\underline{x})$  is sufficient for  $\underline{\theta}$  and its distribution is complete then if there exists a function  $t(s(\underline{x}))$  such that

$$\underline{e}_{\theta}[t(s(\underline{x}))] = \gamma(\underline{\theta})$$

for all  $\underline{\theta}$  (i.e.  $t(s(\underline{x}))$  is unbiased and a function of  $s(\underline{x})$  only) then  $t(s(\underline{x}))$  is the (unique) minimum variance unbiased estimator of  $\gamma(\underline{\theta})$ .

Theorem 1 is essentially due to Lehmann and Scheffé (6) and proofs can be found in various texts, e.g. Lehmann (5), Fraser (4), or Rao (7). Use of Theorem 1 appears limited in that one must find the estimator i.e. no method is implied by the Theorem. The following result due to Rao and Blackwell yields a method for finding  $t(s(\underline{x}))$  (often called "Blackwellization").

Theorem 2. If  $s(\underline{x})$  is a sufficient statistic for  $\underline{\theta}$  and its distribution is complete and if  $t_1(\underline{x})$  is any unbiased estimator for  $\gamma(\underline{\theta})$  then the conditional expectation of  $t_1(\underline{x})$  given  $s(\underline{x})$  is the minimum variance unbiased estimator for  $\gamma(\underline{\theta})$ .

Proofs of theorem 2 can be found in Lehmann, Fraser or Rao among others. To use the result one still needs to find an unbiased estimator for  $\gamma(\underline{\theta})$  but in many applications (e.g. the one considered here) there is a simple choice available and the method reduces to computation of the necessary conditional expectation.

Consider now the estimation of  $F_{\theta}(x_0)$  given that  $X_1, X_2, \dots, X_n$  represents a random sample from the distribution  $F_{\theta}$  having a complete sufficient statistic  $s(\underline{x})$ . Let  $t_1(\underline{x}) = I_{x_0}(X_1)$  be the indicator function of the interval  $(-\infty, x_0]$  i.e.

$$I_{x_0}(x_1) = \begin{cases} 1 & \text{if } x_1 \leq x_0 \\ 0 & \text{otherwise} \end{cases}$$

Then

$$\underline{\mathbb{E}}_{\theta}[I_{x_0}(x_1)] = P_{\theta}[X_1 \leq x_0] = F_{\theta}(x_0)$$

so that  $I_{x_0}(x_1)$  is an unbiased estimator of  $F_{\theta}(x_0)$ . It follows from Theorem 2 that

$$\underline{\mathbb{E}}[I_{x_0}(x_1) | s(x)]$$

is the minimum variance unbiased estimator for  $F_{\theta}(x_0)$ . Similarly if  $F_{\theta}$  is discrete the minimum variance unbiased estimator for  $f_{\theta}(x_0) = P_{\theta}[X = x_0]$  (where  $x_0$  is a "jump" point) of  $F_{\theta}$  is

$$\underline{\mathbb{E}}[\delta_{x_0}(x_1) | s(x)]$$

where

$$\delta_{x_0}(x_1) = \begin{cases} 1 & x_1 = x_0 \\ 0 & \text{otherwise.} \end{cases}$$

For illustrative purposes we indicate the types of calculation for two examples, the Poisson and the normal (known variance).

Example (Poisson): This example can be found in Lehmann (5). Let  $X_1, X_2, \dots, X_n$  be independent Poisson random variables with parameter  $\lambda$ . It is well known that  $S_n = \sum X_i$  is a sufficient statistic for  $\lambda$  and that its distribution is complete.

To estimate  $\gamma(\lambda) = P_{\lambda}[X = j] = \frac{e^{-\lambda} \lambda^j}{j!}$  we form

$$\delta_j(x_1) = \begin{cases} 1 & x_1 = j \\ 0 & \text{otherwise} \end{cases} \quad \text{which is trivially unbiased}$$

and compute  $\underline{\mathbb{E}}[\delta_j(x_1)/S_n]$ . Clearly

$$\underline{\mathbb{E}}[\delta_j(x_1)/S_n] = 0P[\delta_j(x_1) = 0/S_n] + 1P[\delta_j(x_1) = 1/S_n]$$

$$\frac{P[\delta_j(x_1) = 1, S_n = s]}{P[S_n = s]} = \frac{P[X_1 = j, \sum_{i=2}^n X_i = s]}{P[\sum_{i=1}^n X_i = s]}$$

$$= \frac{P[X_1 = j] P[\sum_{i=2}^n X_i = s - j]}{P[\sum_{i=1}^n X_i = s]}.$$

Since it is known that the sum of  $k$  Poisson variables is Poisson with parameter  $k\lambda$  it follows that

$$E[\delta_j(X_1)/S_n] = \frac{[e^{-\lambda} \lambda^j / j!][e^{-(n-1)\lambda} [(n-1)\lambda]^{s-j} / (s-j)!]}{e^{-n\lambda} (n\lambda)^s / s!}$$

$$= \frac{s!}{j!(s-j)!} \left(\frac{1}{n}\right)^j \left(1 - \frac{1}{n}\right)^{s-j}$$

Hence the minimum variance unbiased estimator of  $\frac{e^{-\lambda} \lambda^j}{j!} = P_\lambda(X = j)$  is

$$\left(\frac{S_n}{n}\right) \left(\frac{1}{n}\right)^j \left(1 - \frac{1}{n}\right)^{S_n-j}$$

where  $S_n = \sum_{i=1}^n X_i$ .

Example (Normal): Let  $X_1, X_2, \dots, X_n$  be independent normal random variables with mean  $\mu$  and known variance  $\sigma^2$ . Then  $\bar{X}$  is a sufficient statistic with a complete distribution. Thus to estimate

$$F_\mu(x_0) = P_\mu(X \leq x_0) = \int_{-\infty}^{x_0} \frac{e^{-(x-\mu)^2/2\sigma^2}}{\sigma\sqrt{2\pi}} = \Phi\left(\frac{x_0 - \mu}{\sigma}\right)$$

we simply need to evaluate

$$E[t_1(X_1)/\bar{X}] = P[X_1 \leq x_0/\bar{X}]$$

where  $t_1(x_1) = \begin{cases} 1 & x_1 \leq x_0 \\ 0 & \text{otherwise} \end{cases}$

It is clear that  $X_1$  and  $\bar{X}$  are jointly normal with mean vector  $(\mu, \mu)$  and covariance matrix

$$\sigma^2 \begin{bmatrix} 1 & \frac{1}{n} \\ \frac{1}{n} & \frac{1}{n} \end{bmatrix}.$$

From the usual theory of the multivariate normal distribution the conditional distribution of  $X_1$  given  $\bar{X}$  is thus  $N(\mu + (\bar{x} - \mu), \sigma^2(1 - \frac{1}{n})) = N(\bar{x}, \sigma^2(1 - \frac{1}{n}))$  so that

$$\begin{aligned} P[X_1 \leq x_0 | \bar{x}] &= \int_{-\infty}^{x_0} \frac{e^{-(x_1 - \bar{x})^2/2\sigma^2(1 - \frac{1}{n})}}{\sigma(1 - \frac{1}{n})^{1/2} \sqrt{2\pi}} dx_1 \\ &= \Phi \left[ \frac{\sqrt{n}(x_0 - \bar{x})}{\sigma\sqrt{n-1}} \right] \end{aligned}$$

Hence the minimum variance unbiased estimator of  $\Phi(\frac{x_0 - \mu}{\sigma})$  is  $\Phi \left[ \frac{\sqrt{n}}{\sigma\sqrt{n-1}} (x_0 - \bar{x}) \right]$ .

In table 1 we have compiled some of the estimators for probabilities which have appeared in the literature (the compilation is due most recently to Pierce et al. (3) and we follow their notation). In addition the upper and lower bounds for the variance of the estimators which will be discussed in section 3 are tabled. The calculation involved in obtaining these estimators is the same in principle as for the examples presented.

Looking at the published results, as previously mentioned, indicates that no attention has been given to obtaining the variances (and/or obtaining some form of confidence interval) for the estimators of table 1 and similar type estimators. An example quickly illuminates the type of difficulty encountered. Consider the variance of the estimator for  $P_\lambda(X = j)$  in the Poisson example. Since the expectation squared is known to be  $(e^\lambda \lambda^j / j!)^2$  we need only to evaluate the expectation of  $(\frac{j!}{n!} (\frac{\lambda}{n})^j (1 - \frac{\lambda}{n})^{n-j})^2$  squared which is

$$\sum_{s=0}^{\infty} \binom{s}{j}^2 \left(\frac{1}{n}\right)^{2j} \left(1 - \frac{1}{n}\right)^{2(s-j)} \frac{e^{-n\lambda} (n\lambda)^s}{s!}$$

a formidable problem for analytic purposes. Similar difficulties are present for the other estimators. It would appear useful to obtain numerical results for the estimators of table one and/or approximate expressions for the variances. The problem is not without practical value since many problems often reduce to estimation of a probability or distribution function and information on the precision of such estimates is desirable. In the next section simple upper and lower bounds are obtained for the variances of estimators of the type considered in table 1.

### 3. Bounds on variances of the estimators and some open problems

In this section the Cramér-Rao lower bound (where applicable) is obtained for the variance of estimators of the type in table 1 and a crude upper bound for these variances is also obtained. Presumably wide separation between these bounds for a particular estimator would indicate the need for more subtle bounds and/or numerical work of the type indicated in section 2.

If the necessary regularity conditions are fulfilled (Rao(7)) the generalized Cramér-Rao Inequality states that

$$\text{Var}_{\underline{\theta}}[t(\underline{x})] \geq \sum_i \sum_j I^{i,j} \frac{\partial \gamma(\underline{\theta})}{\partial \theta_i} \frac{\partial \gamma(\underline{\theta})}{\partial \theta_j}$$

where  $I^{i,j}$  is the  $i - j$  element of the inverse of the information matrix with  $i=j$  element

$$I_{i,j} = n \frac{\partial^2 \log f_{\underline{\theta}}(\underline{x})}{\partial \theta_i \partial \theta_j}$$

and  $t(\underline{x})$  is any unbiased estimator of  $\gamma(\underline{\theta})$ .

If one considers the Poisson distribution we have that

$$f_{\underline{\theta}}(\underline{x}) = e^{-\lambda} \lambda^{\underline{x}} / \underline{x}!$$

so that

$$\frac{\partial^2}{\partial \theta_i \partial \theta_j} \left[ \log n f_{\theta}(x) \right] = + \frac{1}{\lambda}.$$

Hence  $I^{i,j}$  is a scalar, namely  $\lambda/n$ . If we wish to estimate  $\gamma(\lambda) = e^{-\lambda} \lambda^j/j!$  we have

$$\begin{aligned} \frac{\partial \gamma(\lambda)}{\partial \lambda} &= \frac{e^{-\lambda} \lambda^{j-1}}{j!} - \frac{e^{-\lambda} \lambda^j}{j!} \\ &= \frac{e^{-\lambda} \lambda^j}{j!} [\frac{j}{\lambda} - 1] \\ &= \gamma(\lambda) [\frac{j}{\lambda} - 1] \end{aligned}$$

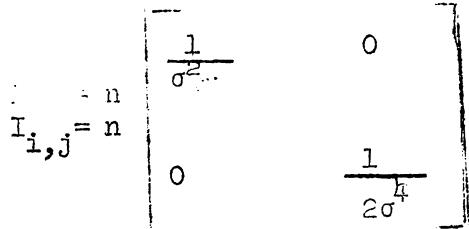
so that the lower bound to the variance is

$$\frac{\gamma(\lambda)^2 \lambda}{n} [\frac{j}{\lambda} - 1]^2.$$

As another example consider the normal distribution with mean  $\mu$  and variance  $\sigma^2$ . Then

$$f_{\theta}(x) = (2\pi)^{-\frac{1}{2}} (\sigma^2)^{-\frac{1}{2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

and



so that



If we wish to estimate  $P_{\underline{\theta}}(X \leq x_0) = \Phi\left(\frac{x_0 - \mu}{\sigma}\right) = \gamma(\underline{\theta})$  we have that

$$\frac{\partial \gamma(\underline{\theta})}{\partial x} = -\frac{1}{\sigma} \Phi' \left( \frac{x_0 - \mu}{\sigma} \right)$$

$$\frac{\partial \gamma(\underline{\theta})}{\partial \sigma^2} = - \left[ \Phi' \left( \frac{x_0 - \mu}{\sigma} \right) \right] \left( \frac{1}{2} \right) (\sigma^2)^{-3/2} (x_0 - \mu)$$

Hence the lower bound is

$$\begin{aligned} & \left( \frac{1}{n} \right) \left\{ \left[ \Phi' \left( \frac{x_0 - \mu}{\sigma} \right) \right]^2 + \left( \frac{1}{2} \right) (x_0 - \mu)^2 \left[ \Phi' \left( \frac{x_0 - \mu}{\sigma} \right) \right]^2 \frac{1}{\sigma^2} \right\} \\ &= \left( \frac{1}{n} \right) \left[ \Phi' \left( \frac{x_0 - \mu}{\sigma} \right) \right]^2 \left\{ 1 + \frac{1}{2} \left[ \frac{x_0 - \mu}{\sigma} \right]^2 \right\}. \end{aligned}$$

If we are estimating probabilities we know that

$t_{x_0}(x_i) = \begin{cases} 1 & X_i \leq x_0 \\ 0 & \text{otherwise} \end{cases}$  is an unbiased estimator. Moreover its variance is clearly  $F_{\underline{\theta}}(x_0)[1 - F_{\underline{\theta}}(x_0)]$  since

$$\underline{\epsilon}_{\underline{\theta}}[t_{x_0}(x)]^2 = P_{\underline{\theta}}[X_i \leq x_0] = F_{\underline{\theta}}(x_0).$$

Hence  $\frac{1}{n} \sum_{i=1}^n t_{x_0}(x_i)$  is an unbiased estimator of  $F_{\underline{\theta}}(x_0)$  with variance

$$\left( \frac{1}{n} \right) F_{\underline{\theta}}(x_0)[1 - F_{\underline{\theta}}(x_0)].$$

In the examples considered in table 1 we know the estimator given has minimum variance so that an upper bound to its variance is simply

$$\left( \frac{1}{n} \right) F_{\underline{\theta}}(x_0)[1 - F_{\underline{\theta}}(x_0)].$$

A similar result holds when  $F$  is discrete. The upper bound then becomes

$$\left(\frac{1}{n}\right) f_{\theta}(j)[1 - f_{\theta}(j)] .$$

In the Poisson example  $f_{\theta}(j) = \frac{e^{-\lambda} \lambda^j}{j!} = \gamma(\lambda)$  so that an upper bound is

$$\left(\frac{1}{n}\right) \gamma(\lambda)[1 - \gamma(\lambda)]$$

while in the normal example an upper bound is

$$\left(\frac{1}{n}\right) \Phi\left(\frac{x_0 - \mu}{\sigma}\right)[1 - \Phi\left(\frac{x_0 - \mu}{\sigma}\right)] .$$

It is rather obvious that the upper bound is indeed crude but it provides some information about the variance.

Clearly work needs to be done on finding exact variances of the estimators in table 1 either analytically or numerically. In lieu of analytic results sharper upper bounds could perhaps be developed. In one special case, at least, one can find the exact variance and it is of some interest to indicate the relationship of the exact variance to the bounds above. In the Poisson example if  $j = 0$  we want to estimate  $e^{-\lambda} = P_{\lambda}[X = 0] = \gamma(\lambda)$  so that the Cramér-Rao lower bound to the variance is

$$\frac{\lambda e^{-2\lambda}}{n}$$

while an upper bound to the variance is

$$\frac{e^{-\lambda}[1 - e^{-\lambda}]}{n} .$$

The minimum variance estimator is from table 1 given by

$$(1 - \frac{1}{n}) S_n$$

where  $S_n = \sum_{i=1}^n x_i$ . Hence

$$\begin{aligned}
 \varepsilon_\lambda [1 - \frac{1}{n}]^{2s} &= \sum_{s=0}^{\infty} (1 - \frac{1}{n})^{2s} \frac{e^{-n\lambda} (n\lambda)^s}{s!} = e^{-n\lambda} \sum_{s=0}^{\infty} \frac{[(1 - \frac{1}{n})^2 n\lambda]^s}{s!} \\
 &= e^{-n\lambda} e^{(1 - \frac{1}{n})^2 n\lambda} \\
 &= e^{-2\lambda + \frac{\lambda}{n}}.
 \end{aligned}$$

It follows that the variance of the minimum variance estimator is

$$e^{-2\lambda} [e^{\lambda/n} - 1]$$

which approaches the lower bound as  $n^{-2}$ . The rapid approach to the lower bound would suggest approximating the variance of the minimum variance estimator with the Cramér-Rao lower bound and leads one to the problem of specifying the class of distributions and/or parametric functions for which the variance of the minimum variance estimator approaches the Cramér-Rao lower bound as  $n^{-2}$ . Another problem would be investigation of the distribution of the estimators in table 1.

Table 1.

Distribution	Estimand	Estimator	Lower Bound	Upper Bound
$N(\mu, \sigma^2)$ $\mu$ unknown $\sigma^2$ known	$\Phi\left(\frac{x_0 - \mu}{\sigma}\right)$	$\Phi\left(\frac{\sqrt{n}(\bar{x} - \mu)}{\sqrt{n-1}}\right)$	$\left[\frac{\Phi^2\left(\frac{x_0 - \mu}{\sigma}\right)}{n}\right]^2$	$\Phi\left(\frac{x_0 - \mu}{\sigma}\right)\left[1 - \Phi\left(\frac{x_0 - \mu}{\sigma}\right)\right]$
$N(\mu, \sigma^2)$ $\mu$ known $\sigma^2$ unknown	$\Phi\left(\frac{x_0 - \mu}{\sigma}\right)$	0 if $x_0 < \mu - \sqrt{\frac{n-2}{n}}\sigma$ 1 if $x_0 > \mu + \sqrt{\frac{n-2}{n}}\sigma$ $F_{t, n-1} \left\{ \frac{(n-1)^{\frac{1}{2}}(x_0 - \mu)}{[n\sigma^2 - (x_0 - \mu)^2]^{\frac{1}{2}}} \right\}$ otherwise	$\frac{(x_0 - \mu)^2}{2n\sigma^2} \left[ \Phi'\left(\frac{x_0 - \mu}{\sigma}\right) \right]^2$	$\Phi\left(\frac{x_0 - \mu}{\sigma}\right)\left[1 - \Phi\left(\frac{x_0 - \mu}{\sigma}\right)\right]$
$N(\mu, \sigma^2)$ $\mu$ unknown $\sigma^2$ unknown		0 if $x_0 < \bar{x} - (n-1)s/\sqrt{n}$ 1 if $x_0 > \bar{x} + (n-1)s/\sqrt{n}$ $F_{t, n-2} \left\{ \left[ \frac{(n-2)n}{2} \left( \frac{x_0 - \bar{x}}{s} \right) / \left[ (n-1)^2 s^2 - n(x_0 - \bar{x})^2 \right] \right]^{\frac{1}{2}} \right\}$ otherwise	$\frac{1}{n} \left[ 1 + \left( \frac{x_0 - \mu}{2\sigma} \right)^2 \right] \cdot \left[ \Phi'\left(\frac{x_0 - \mu}{\sigma}\right) \right]^2$	$\Phi\left(\frac{x_0 - \mu}{\sigma}\right)\left[1 - \Phi\left(\frac{x_0 - \mu}{\sigma}\right)\right]$
Poisson	$\frac{e^{-\lambda} \lambda^j}{j!}$	$\begin{cases} \binom{s}{j} \left(\frac{1}{n}\right)^j \left(1 - \frac{1}{n}\right)^{s-j} & \text{if } j \leq s \\ 0 & \text{if } j > s \end{cases}$	$\frac{e^{-2\lambda} \lambda^{2j-1} (j-\lambda)^2}{n(j!)^2}$	$\frac{-\lambda \lambda^j}{j!} \left[ 1 - \frac{e^{-\lambda} \lambda^j}{j!} \right]$

Distribution	Estimand	Estimator	Lower Bound	Upper Bound
Binomial (Sample of size N)	$\binom{n}{j} p^j (1-p)^{n-j}$	$\frac{\binom{n}{j} \left( \frac{nN - n}{S_N - j} \right)}{\binom{nn}{S_N}}$ if $j \leq S_N$ $j > S_N$	$\frac{(j) p^{2j-1} (1-p)^{2(n-j)-1}}{nN} \frac{(j-np)^2}{(j-np)^2}$	$\frac{\binom{n}{j} p^j (1-p)^{n-j} \left[ 1 - \left( \frac{n}{j} \right) p^j (1-p)^{n-j} \right]}{N}$
Exponential	$\int_0^{x_0} \lambda e^{-\lambda t} dt$ 0 $x_0 < 0$ 1 $x_0 > S_n$ $1 - \left( 1 - \frac{x_0}{S_n} \right)^{n-1} \quad 0 \leq x_0 \leq S_n$		$\frac{(x_0 \lambda)^2 e^{-2x_0 \lambda}}{n}$	$\frac{e^{-x_0 \lambda} \left[ 1 - e^{-x_0 \lambda} \right]}{n}$

## 4. Table I

Notations used in Table I.

$\Phi$  - cumulative standard normal

$$\hat{\sigma}^2 = \left( \frac{1}{n} \right) \sum_{i=1}^n (x_i - \bar{x})^2$$

$$S = \sum_{i=1}^n (x_i - \bar{x})^2$$

$$S_n = \sum_{i=1}^n x_i$$

$F_{t, n-2}$  - cumulative t with  $n-2$  degrees of freedom

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