Biometrika (1980), 67, 3, pp. 715-8
Printed in Great Britain

## Variance estimation for the second-order jackknife

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### SUMMARY

This paper considers Sharot's family of jackknives (1976) and chooses a member of it using a minimum variance based criterion. The criterion is different from that considered by Sharot, which is claimed to be inappropriate. Results on the variance estimator of the jackknife are derived and compared with those of Hinkley (1978). A Monte Carlo simulation study supports the above conclusion.

Some key words: Correlation; Jackknife; Influence function; Variance reduction.

#### 1. Introduction

The jackknife is a well-known method for bias reduction and robust interval estimation. An excellent review is given by Miller (1974). Let  $x_1, ..., x_n$  be independent and identically distributed random variables with cumulative distribution function  $F(x, \theta)$ . Let  $T_n = T_n(x_1, ..., x_n)$  be an estimator of  $\theta$  based on n observations. Define  $T_{-i}$  and  $T_{-i-j}$  to be estimators of  $\theta$  based on all but the ith observation and on all but the ith and jth observation respectively. If we write

$$\overline{T}_{\cdot} = n^{-1} \sum T_{-i}, \quad \overline{T}_{\cdot \cdot} = 2\{n(n-1)\}^{-1} \sum_{i < j} T_{-i-j} \quad (i < j),$$

$$g_{i} = nT_{n} - (n-1)T_{-i} \quad (i = 1, ..., n),$$

then the first- and second-order jackknives are

$$\hat{\theta}^{(1)} = n^{-1} \sum g_i, \quad \hat{\theta}^{(2)} = \frac{1}{2} \{ n^2 T_n - 2(n-1)^2 \overline{T}_1 + (n-2)^2 \overline{T}_1 \},$$

respectively. Sharot (1976) suggested the family of jackknives

$$J(p) = 2\{n(n-1)\}^{-1} \sum_{i=1}^{n} \sum_{j=1}^{n} g_{ij}(p)$$
 (1·1)

with variance estimator of J(p)

$$S_J^2(p) = 4\{n(n-1)(n-2)\}^{-1} \sum_{i=1}^n \sum_{j=1}^n \{g_{ij}(p) - J(p)\}^2, \qquad (1\cdot 2)$$

where for i < j

$$g_{ij}(p) = pnT_n + \frac{1}{2}(1-2p)(n-1)(T_{-i} + T_{-j}) + (p-1)(n-2)T_{-i-j}. \tag{1.3}$$

Sharot suggested the choice of  $J(p^*)$ , where  $p^*$  is the value of p minimizing  $S_J^2(p)$ . In §2 of this paper we show, extending work of Hinkley (1978), that the  $g_{ij}(p)$  are substantially correlated and therefore  $S_J^2(p)$  is inappropriate as a variance estimator of J(p). In §3 we derive asymptotically unbiased estimators of the variance of first- and second-order influence functions to find the variance of  $g_{ij}(p)$ , In §§ 4 and 5 we propose a rule for choosing a member from Sharot's family and we investigate the above results by a simulation study.

### 2. DERIVATION OF THE COVARIANCE MATRIX OF THE $g_{ij}(p)$

Suppose that  $T_n$  is a regular differentiable functional of the form  $T_n = t(\hat{F}_n)$ , where  $\hat{F}_n$  is the empirical distribution function. Then  $\theta = T(F)$  and, following Hinkley (1978), we have that

$$T_n \sim \theta + n^{-1} \sum_{j=1}^n f_1(x_j) + \frac{1}{2} n^{-2} \sum_{j=1}^n \sum_{l=1}^n f_2(x_j, x_l),$$
 (2.1)

where  $f_1(x)$ ,  $f_2(x,y)$  are the first- and second-order influence functions of T (Hampel, 1974), defined by the identities

$$\begin{split} \left[\frac{d}{d\varepsilon} T\{(1-\varepsilon) F + \varepsilon F_1\}\right]_{\varepsilon=0} &= \int f_1(x) dF_1(x), \\ \left[\frac{d^2}{d\varepsilon^2} T\{(1-\varepsilon) F + \varepsilon F_1\}\right]_{\varepsilon=0} &= \int \int f_2(x,y) dF_1(x) dF_1(y), \end{split} \tag{2.2}$$

where  $F_1$  is an arbitrary cumulative distribution function. We write

$$(i) = f_1(x_i)$$
  $(i = 1, ..., n),$   $(i, j) = f_2(x_i, x_j)$   $(i, j = 1, ..., n).$ 

A detailed analysis of  $g_{ij}(p)$  using all terms given in (2·1) gives

$$g_{ij}(p) \sim \theta + \frac{1}{2}(i) + \frac{1}{2}(j) + T_1(i,j),$$
 (2.3)

where

$$T_1(i,j) = a_1 \left[ 2n^{-1} \sum_{l=1}^n \left\{ \sum_{m=1}^n (m,l) - n(l,i) - n(l,j) \right\} + (i,i) + (j,j) \right] + a_2(i,j)$$

and  $a_1 = (2p-n)/\{4(n-1)(n-2)\}$ ,  $a_2 = (p-1)/(n-2)$ . We define  $\sigma_{11} = \text{var}\{(i)\}$ ,  $\sigma_{22} = \text{var}\{(i,l)\}$   $(i \neq l)$  and we choose p = kn, where k is a constant, independent of n. This means that asymptotically we are working with a family of jackknives more like a second-order jackknife, because  $\hat{\theta}^{(1)} = J(1)$ ,  $\hat{\theta}^{(2)} = J(\frac{1}{2}n)$ . After some algebra we find from  $(2\cdot 3)$ , omitting terms of o(1/n), that

$$\begin{aligned} \operatorname{var} \left\{ g_{ij}(p) \right\} &= \tfrac{1}{2} \sigma_{11} + k^2 \sigma_{22} \quad (i \neq j), \quad \operatorname{cov} \left\{ g_{ij}(p), g_{il}(p) \right\} = \tfrac{1}{4} \sigma_{11} \quad (i < j, \ i < l, \ l \neq j), \\ & \operatorname{cov} \left\{ g_{ij}(p), g_{li}(p) \right\} = \tfrac{1}{4} \sigma_{11} \quad (i < j, \ l < i, \ l \neq j), \\ & \operatorname{cov} \left\{ g_{ij}(p), g_{lm}(p) \right\} = 0 \quad (i < j; \ l < m; \ l \neq i, j; \ m \neq i, j). \end{aligned}$$

Expressions (2·4) reveal that asymptotically there is nonzero correlation between some of the  $g_{ij}(p)$ . Using (2·4) and the definitions of J(p) and  $S_J^2(p)$  we find that

$$\operatorname{var}\left\{J(p)\right\} = n^{-1}(\sigma_{11} + 2k^2n^{-1}\sigma_{22}), \quad E\{S_J^2(p)\} \sim n^{-1}(\sigma_{11} + 2k^2\sigma_{22}), \tag{2.5}$$

so that Sharot's estimator is positively biased asymptotically, when p is chosen to give something like a second-order jackknife. In his paper Sharot suggests choosing p to minimize  $S_J^2(p)$ . One can see from the results presented here that the effect of this procedure is to move p away from values close to the second-order jackknife towards those similar to the first-order jackknife. This is due to the positive bias of  $S_J^2(p)$  for large p, and its lack of bias for p=1. The choice of p by this criterion is not based on any valuable property of J(p), but simply gets rid of p values for which  $S_J^2(p)$  is badly biased. Only if  $\sigma_{22}$  is very small compared with  $\sigma_{11}$  would  $S_J^2(p)$  be a good estimator of var  $\{J(p)\}$  for p of order n.

# 3. New estimators of $\sigma_{11}$ and $\sigma_{22}$ unblased to the first order

Hinkley (1978) estimates  $\sigma_{11}$ ,  $\sigma_{22}$  by the corresponding sample moments of the estimators of (i) and (i,j) for  $i \neq j$ . Using  $(2\cdot 1)$  we find that his estimator of  $\sigma_{22}$  is biased to o(1/n)

because

$$\operatorname{var}\left\{(i,j)^*\right\} \sim \sigma_{22} - 4n^{-1}\sigma_{22}, \quad \operatorname{cov}\left\{(i,i-1)^*,(i-1,i-2)^*\right\} \sim -2n^{-1}\sigma_{22},$$

where  $(i,j)^*$  is the estimator of (i,j). Further estimators of  $\sigma_{11}$ ,  $\sigma_{22}$  can be found by choosing that quadratic form in  $g_{ij}(p)$  which treats the  $g_{ij}(p)$  symmetrically and is unbiased to the first order. Using  $(2\cdot 4)$  we find the estimators

$$\begin{split} \hat{\sigma}_{11} &= 4\{n(n-1)\,(n-2)\}^{-1}S_2 - 16\{n(n-1)\,(n-2)\,(n-3)\}^{-1}S_3, \\ \hat{\sigma}_{22} &= 2\{k^2n(n-1)\}^{-1}S_1 - 2\{k^2n(n-1)\,(n-2)\}^{-1}S_2 + 4\{k^2n(n-1)\,(n-2)\,(n-3)\}^{-1}S_3, \end{split} \tag{3.1}$$

where

$$\begin{split} S_2 &= \sum_{i < j < l} \{g_{ij}(p) \, g_{il}(p) + g_{il}(p) \, g_{jl}(p) + g_{ij}(p) \, g_{jl}(p) \}, \quad S_1 = \sum_{i < j} g_{ij}^2(p), \\ S_3 &= \sum_{i < j < k < l} \{g_{ij}(p) \, g_{kl}(p) + g_{ik}(p) \, g_{jl}(p) + g_{jk}(p) \, g_{il}(p) \}. \end{split}$$

To the first order  $E(\hat{\sigma}_{11}) = \sigma_{11}$ ,  $E(\hat{\sigma}_{22}) = \sigma_{22}$ . The estimators  $\hat{\sigma}_{11}$  and  $\hat{\sigma}_{22}$  are, to the first order, minimum norm quadratic unbiased estimators, minimum, of  $\sigma_{11}$  and  $\sigma_{22}$  (Rao, 1972).

#### 4. REDUCTION OF VARIANCE ESTIMATOR IN A NEW JACKKNIFE

One might think, as did Sharot, of choosing k to minimize  $\hat{\sigma}_{11}$  and so consequently  $\text{var}\{J(p)\}$  in  $(2\cdot 5)$ , to the first order. Another possible choice of p is to minimize the variance of  $\hat{\sigma}_{11}$ . If we assume that the  $g_{ij}(p)$  are asymptotically multivariate normal and use  $(2\cdot 4)$ , the best choice of k is zero to the first order. In the simulations of §5 only the case k=0 is considered since the computation of p to minimize  $\hat{\sigma}_{11}$  is complicated and the results in the case k=0 are clearly better.

### 5. Monte Carlo simulation studies

We consider estimation from the negative exponential distribution with probability density function  $f(x,\theta) = \theta e^{-\theta x}$  and cumulative distribution function  $F(x,\theta)$ . We estimate  $\theta$  by  $\bar{x}^{-1} = \{\int x d\hat{F}_n(x)\}^{-1}$ . Then,  $\theta = T(F) = \{\int x dF(x)\}^{-1}$ . For the functional  $\theta = T(F)$  we find from (2.2)

$$f_1(x) = \theta(1-\theta x), \quad f_2(x,y) = 2\theta(1-\theta x)(1-\theta y), \quad \sigma_{11} = E_F(f_1^2) = \theta^2, \quad \sigma_{22} = E_F(f_2^2) = 4\theta^2. \tag{5.1}$$

For each of n=12, 24, 30, 40, 50, 60, 10,000 samples are generated from the negative exponential distribution with mean  $\mu_x=1$ , on the CDC7600 of London University. Our aim is to compare the performances of the following two members of Sharot's family J(p) of estimators:  $\hat{J}^{(1)} = J(p)$  with p=0 and  $J(p^*)$  with  $p^*$  chosen to minimize  $S_J^2(p)$ . We choose as a 'yardstick' the minimum variance unbiased estimator:  $\tilde{\theta} = (n-1)n^{-1}\tilde{x}^{-1}$ . The results are summarized in Tables 1 and 2.

Table 1. Estimation of  $\theta = 1$  in negative exponential distribution

	Performance of $\hat{J}^{(1)}$ , $J(p^*)$				Variance estimator $S_J^2(p)$				
n	Estimator	Mean	Rel. var.	Rel. MSE	$oldsymbol{\sigma^2}$	$\sigma_J^2$	$E\{S_J^2(p)\}$	St. dev. of $S_J^2(p)$	$[\mathtt{MSE}~\{S_J^2(p)\}]^{rac{1}{2}}$
12	$\hat{J}^{(1)} \ J(p^*)$	0·989 0·987	$1.017 \\ 1.022$	$\begin{array}{c} 1 \cdot 019 \\ 1 \cdot 024 \end{array}$	$\begin{array}{c} 0.084 \\ 0.174 \end{array}$	$\begin{array}{c} 0 \cdot 103 \\ 0 \cdot 104 \end{array}$	$0.117 \\ 0.147$	$0.181 \\ 0.205$	$0.182 \\ 0.209$
24	$\hat{J}^{(1)} \ J(p^*)$	$1.002 \\ 1.002$	1.003 $1.004$	$1.004 \\ 1.005$	$0.042 \\ 0.065$	$\begin{array}{c} 0.047 \\ 0.048 \end{array}$	$0.048 \\ 0.055$	$\begin{array}{c} 0 \cdot 004 \\ 0 \cdot 040 \end{array}$	0·004 0·041
40	$\hat{J}^{(1)} \ J(p^*)$	1·000 1·000	1·001 1·001	1·001 1·001	$0.025 \\ 0.033$	$0.028 \\ 0.028$	$0.029 \\ 0.030$	$0.001 \\ 0.016$	0·001 0·016
60	$\hat{J}^{(1)} \ J(p^*)$	1·000 1·000	$1.000 \\ 1.000$	1·000 1·000	$0.017 \\ 0.020$	$0.017 \\ 0.018$	0·018 0·019	0·007 0·008	$\begin{array}{c} 0.007 \\ 0.008 \end{array}$

Table 2. 95% large sample confidence intervals for the estimators  $\hat{J}^{(1)}$ ,  $J(p^*)$  and their variances

$\boldsymbol{n}$	Estimator	Means of estimators	$E\{S_J^2(p)\}$
12	$\hat{J}^{(1)} \ J(p^*)$	(0.979, 0.992) (0.982, 0.995)	(0.144, 0.120) (0.142, 0.150)
24	$\hat{J}^{(1)} \ J(p^*)$	(0.996, 1.004) (0.996, 1.005)	(0.047, 0.049) (0.053, 0.055)
40	$\hat{J}^{(1)}$ $J(p^*)$	(0.997, 1.003) (0.997, 1.004)	(0.028, 0.030) (0.029, 0.030)
60	$\hat{J}^{(1)}$ $J(p^*)$	(0·997, 1·002) (0·997, 1·002)	(0·017, 0·019) (0·018, 0·019)

From Table 1 we find that the estimator  $J^{(1)}$  is superior to  $J(p^*)$  with respect to bias, variance and mean squared error. The column  $\sigma^2$  represents the true population variance to  $o(n^{-1})$  for each of the estimators and is  $n^{-1}(\sigma_{11} + 2k^2n^{-1}\sigma_{22}) = n^{-1}(\sigma_{11} + 2p^2n^{-3}\sigma_{22})$ , where we find from (5·1) that  $\sigma_{11} = 1$ ,  $\sigma_{22} = 4$ ; the sampling variance for each of the estimators over 10,000 samples is  $\sigma_J^2$ . We may compare  $\sigma^2$  and  $\sigma_J^2$  with the corresponding estimators of the expected value of the variance estimators, labelled  $E\{S_J^2(p)\}$  in the table. The variance estimators are given from (1·2) for the estimator  $J(p^*)$  and from (2·5) for  $J^{(1)}$ , with (3·1) used for calculation of  $\sigma_{11}$  and  $\sigma_{22}$ . The conclusions from Table 1 are that, for every value of n considered, the variance estimator of  $J^{(1)}$  is less biased and has less standard deviation and mean squared error than the variance estimator of  $J(p^*)$ . Hence, the estimator  $J^{(1)} = J(p)$  with p = 0 is more efficient than Sharot's estimator  $J^{(2)}$ .

Table 2 contains 95% large sample confidence intervals for the mean and the variance of

the estimators  $\hat{J}^{(1)}$  and  $J(p^*)$ .

Additional research is needed on the relation between Hinkley's and MINQUE estimators of  $\sigma_{11}$  and  $\sigma_{22}$  as n increases.

The author would like to thank Dr M. Knott for his very valuable help throughout the preparation of this paper. Helpful comments from a referee were also gratefully received.

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[Received October 1979. Revised April 1980]