Nonparametric estimation of the generalized variance

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NONPARAMETRIC ESTIMATION OF THE GENERALIZED VARIANCE

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Summary:

For multivariate distributions with finite second order moments, a nonparametric symmetric, unbiased estimator of the generalized variance is considered, and it is shown to be (nonparametric) optimal for the class of distributions having finite fourth order moments. A jackknifed version of the sample generalized variance is also considered as a contender; it is computationally more convenient and asymptotically equivalent to the former. It is also shown that the second estimator performs quite well (in large sample) relative to the optimal normal theory estimators under several loss functions.

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Running head: Estimation of Generalized Variance.
1. INTRODUCTION

Let \( x_1, \ldots, x_n \) be \( n \) independent and identically distributed random vectors (i.i.d.r.v.) with a distribution function (d.f.) \( F \) defined on the \( p \times 1 \) dimensional Euclidean space \( \mathbb{R}^p \). We assume that \( F \in \mathcal{F} = \{ F : \int \| x \|^2 dF(x) < \infty \} \). The parameter of interest \( \theta \) is the generalized variance \( |\Sigma| \), where

\[
\Sigma = E_F \{(x - Ex)(x - Ex)'\}
\]

and \( |\cdot| \) stands for the determinant. A good amount of work has been done on the estimation of \( \theta \) when \( F \) is assumed to be a multinormal d.f.; the approach has mainly been decision theoretic and the main result states that the best multiple of the sample generalized variance can be improved on (in terms of risk) by using testimators [c.f. Stein (1964), Shorrock and Zidek (1976), Sinha (1976), Sinha and Ghosh (1986), and others], although the amount of improvement is marginal in most cases.

An alternative nonparametric approach to the estimation of \( \theta \) is considered here. In Section 2, a symmetric, unbiased nonparametric estimator is derived and its optimality is established through the use of Hoeffding's (1948) U-statistics theory. A second estimator based on jackknifing on the sample generalized variance is found to be computationally more convenient and asymptotically equivalent to the former nonparametric estimator of \( \theta \). Like the other (improved) parametric estimators, the second nonparametric estimator also comes out as a multiple of the sample generalized variance, and it performs quite well (at least, for large samples) compared to the optimal normal theory estimators under several loss functions (vide Section 3). Thus, the jackknifed estimator seems to enjoy the parametric affinity and nonparametric robustness in broad setup. The former nonparametric estimator is, however, somewhat computationally involved (particularly, for large \( n \)). Finally, in Section 4, some concluding remarks about estimation of \( |\Sigma|^{1/p} \) are made.

2. MAIN RESULTS

Let \( x_1, \ldots, x_n \) be \( n \) independent and identically distributed (i.i.d.) random vectors (r.v.) with a distribution function (d.f.) \( F \), defined on \( \mathbb{R}^p \), for some
It is assumed that
\[ F \in \mathcal{F} = \{ F : \int \|x\|^2 dF(x) < \infty \}, \tag{2.1} \]
where \( \| \cdot \| \) stands for the Euclidean norm. Our goal is to estimate the functional (the generalized variance)
\[ \Theta(F) = |\Sigma(F)| = |E_F((x - Ex)(x - Ex)^t)|, \tag{2.2} \]
where \( |A| \) stands for the determinant of the matrix \( A \). Note that when \( F \) is a multinormal d.f. with unknown mean vector \( \mu \) and dispersion matrix \( \Sigma \), then \( \Theta(F) = |F| \) is typically estimated by \( \hat{\Theta}_n = |S_n| \), where
\[ S_n = (n - 1)^{-1} \sum_{i=1}^n (x_i - \bar{x}_n)(x_i - \bar{x}_n)^t \text{ and } \bar{x}_n = \frac{1}{n} \sum_{i=1}^n x_i. \tag{2.3} \]

To motivate a nonparametric estimator of \( \Theta(F) \), first, we may note that
\[ \hat{\Theta}_n = n(n - 1)^{-1} \sum_{i=1}^n (x_i - \bar{x}_n)(x_i - \bar{x}_n)^t, \tag{2.4} \]
where
\[ \hat{\Theta}_n = \frac{1}{2} (x - x_2)(x_1 - x_2)^t, \tag{2.5} \]
Further, we may note that
\[ \frac{(n - 1)(n - 2)}{(2)} \sum_{1 \leq i < j \leq n} \hat{\Theta}_n(x_i, x_j) = S_n, \forall n \geq 2. \tag{2.6} \]
Thus, \( S_n \) is an optimal (symmetric, unbiased and minimum risk) nonparametric estimator of \( \Sigma(F) \). However, \( \Theta(F) \) is a polynomial function (of degree \( p \)) in the elements of \( \Sigma(F) \), and hence, it is easy to show that \( |S_n| = \hat{\Theta}_n \) is not unbiased for \( \Theta(F) \), although, the bias of \( \hat{\Theta}_n \) is typically of the order \( n^{-1} \). Our first goal is to consider a symmetric and unbiased nonparametric estimator of \( \Theta(F) \).

Let \( x_j = (x_{1j}, \ldots, x_{pj}), j = 1, \ldots, 2p \) be \( 2p \) vectors and define
\[ \hat{\Theta}_n(x_1, \ldots, x_{2p}) = \frac{1}{2} (x_1 - x_2)(x_1 - x_2)^t, \frac{1}{2} (x_3 - x_4)(x_3 - x_4)^t, \ldots, \frac{1}{2} (x_{2p-1} - x_{2p})(x_{2p-1} - x_{2p})^t \].

Note that for the matrix (of order \( p \times p \)) in the determinant in (2.7), the \( j \)th
column depends only on $x_{2j-1}, x_{2j}$, for $j = 1, \ldots, p$. Thus, for $\phi(x_1, \ldots, x_{2p})$, the $p$ columns of this matrix are stochastically independent. Hence, using the standard expansion for the determinant, it readily follows that

$$F_\| \phi(x_1, \ldots, x_{2p}) \| = |\sigma_{1 \ldots p}| = |\Sigma(F)| = \theta(F), \quad \forall F \in \mathcal{F},$$

(2.8)

where $\sigma_j = (\sigma_{1j}, \ldots, \sigma_{pj})'$ stands for the $j$th column vector of $\Sigma(F)$, for $j = 1, \ldots, p$. Thus, $\phi(x_1, \ldots, x_{2p})$ is a kernel of degree $2p$ (although, it is not a symmetric one), and, hence, following the steps in Hoeffing (1948), a symmetric, unbiased estimator of $\theta(F)$ is obtained (for $n \geq 2p$) as

$$U_n = n^{-[2p]} \sum_{1 \leq i_1 \leq \ldots \leq i_{2p} \leq n} \phi(x_{i_1}, \ldots, x_{i_{2p}}),$$

(2.9)

where

$$n^{-[2p]} = n \ldots n - 2p + 1; \quad n^{-[p]} = (n^{-[p]})^{-1}.$$  

(2.10)

Being a U-statistic, $U_n$ shares the nonparametric unbiasedness and optimality (minimum variance/minimum risk with convex loss functions) properties when $F$ is allowed to vary over a subclass of $\mathcal{F}$ for which the variance or the risk of $U_n$ is properly defined (viz., $F \in \mathcal{F}^*$, where $\mathcal{F}^* = \{F: \int \|x\|^4 dF(x) < \infty\}$). $U_n$ is a symmetric function of $x_1, \ldots, x_n$.

It is interesting to note that for $p \geq 1$, $U_n = |S_n| = \hat{\theta}_n$, and moreover, unlike $\hat{\theta}_n$, $U_n$ is not a sole function of the elements of $S_n$. Thus, in the normal theory case (for $F$), whereas it is possible to choose a positive constant $c_{n,p}$ (depending on $n$ and $p$ ($n \geq p$)), such that $c_{n,p} \hat{\theta}_n$ is unbiased for $\theta(F)$ (and a symmetric function of the sample observations too), $c_{n,p} \hat{\theta}_n$ may not be unbiased for $\theta(F)$ when $F$ is not normal and $p \geq 2$. On the other hand, the proposed nonparametric estimator $U_n$ in (2.9), for $p \geq 2$, involves the matrix $S_n$ as well as some other statistics (having smaller contributions). To make this point clear, consider the simplest case of $p = 2$. We have then

$$U_n = n^{-[4]} \sum_{1 \leq i_1 \leq \ldots \leq i_4 \leq n} \phi(x_{i_1}, x_{i_2}, x_{i_3}, x_{i_4})$$

(2.11)

$$= \frac{n(n-1)(n-2)(n-3)}{n^3} |S_n| + \frac{1}{n^3} R_n$$
where
\[
R_n = n^{-\frac{1}{2}} \sum_{1 \leq i \leq j \leq k \leq n} \phi(x_i, x_j, x_k)
\]
\[
= \frac{1}{4} n^{-\frac{1}{2}} \sum_{1 \leq i \leq j \leq k \leq n} \left| \begin{array}{ccc}
(x_{1i} - x_{1j})^2 & (x_{1i} - x_{1k})(x_{2i} - x_{2k}) \\
(x_{1i} - x_{1j})(x_{2i} - x_{2j}) & (x_{2i} - x_{2k})^2 \\
\end{array} \right|
\]

Note that \( R_n \) is not a sole function of \( S_n \). A very similar treatment holds for general \( p \geq 2 \). Whereas for \( E|S_n| \), we need that \( E\|X\|^2_p < \infty \), for \( E U_{n}(=\theta(F)) \), the second moment suffices.

To explore the relationship between \( U_n \) and \( \hat{\theta}_n \), we note that the von Mises' (1947) functional corresponding to the kernel in (2.7) is given by
\[
\psi_n = \int \ldots \int \phi(x_1, \ldots, x_{2p}) d\Phi_n(x_1) \ldots d\Phi_n(x_{2p})
\]
\[
= n^{-2p} \sum_{i=1}^{n} \sum_{i_2=1}^{n} \phi(x_{i_1}, \ldots, x_{i_{2p}}),
\]
where \( F_n(x) = n^{-\frac{1}{2}} \sum_{i=1}^{n} I(x_i - x) \), \( x \in \text{E}^p \) is the sample d.f. Using the identity that
\[
\sum_{i=1}^{n} \sum_{j=1}^{n} (x_{i} - x_{j})(x_{i} - x_{j})' = 2n \sum_{i=1}^{n} (x_{i} - \bar{x})(x_{i} - \bar{x})',
\]
we immediately obtain from (2.7) and (2.13) that
\[
\psi_n = \left( \frac{n-1}{n} \right)^p |S_n| = (1 - n^{-1})^p \hat{\theta}_n.
\]

Further, \( (S_n, n \geq p) \) is a reversed martingale, so that noting that \( |S_n| \) is a convex function of \( S_n \), we claim that
\[
(\hat{\theta}_n, n \geq p + 1) \text{ is a nonnegative reversed sub-martingale.}
\]

As such, using the reversed submartingale convergence theorem, we immediately conclude that \( \hat{\theta}_n \to \Sigma(F) = \theta(F) \) a.s., as \( n \to \infty \), and hence
\[
|\psi_n - \hat{\theta}_n| = 0(n^{-1}) \text{ a.s., as } n \to \infty.
\]

On the other hand, if we assume that
\[
E_F \phi(x_{i_1}, \ldots, x_{i_{2p}}) < \infty, \quad \forall \ 1 \leq i_1 \leq i_2 \leq \ldots \leq i_{2p} = 2p,
\]
then using the results in Section 3.2 [viz. (3.2.9)] of Sen (1981), it follows that
\[ |U_n - V_n| = O(n^{-1}) \text{ a.s., as } n \to \infty. \] (2.19)
Combining (2.17) and (2.19), we obtain that under (2.18),
\[ |U_n - \hat{\theta}_n| = O(n^{-1}) \text{ a.s., as } n \to \infty. \] (2.20)
Also, by the reversed martingale property of U-statistics, we conclude that
\{U_n, n \geq 2p\} is a reversed martingale. (2.21)

Thus, writing \( \hat{\theta}_n = U_n + (\hat{\theta}_n - U_n) \), we conclude that \( U_n \) represents the reversed martingale component of \( \hat{\theta}_n \), while the sub-martingale component \( (\hat{\theta}_n - U_n) \) is \( O(n^{-1}) \) a.s. This can be interpreted as the asymptotic optimality and robustness of \( \hat{\theta}_n = |S_n| \) for estimating \( \theta(F) \), for possibly non-normal \( F \). This decomposition along with (2.20) may also be utilized in the motivation of a jackknifed version of \( \hat{\theta}_n \), which would reduce the bias without compromising the (first order) asymptotic optimality.

To pose this jackknifed version \( \hat{\theta}^*_n \) of \( \hat{\theta}_n \), we define
\[
S_{n-1}^{(i)} = (n-1)^{-1} \sum_{\alpha=1}^{n} (x_{\alpha} - x_{n-1}^{(i)})(x_{\alpha} - x_{n-1}^{(i)}),
\]
(2.22)
\[
x_{n-1}^{(i)} = (n - 1)^{-1} \sum_{\alpha=1}^{n} (x_{\alpha} - x_{n-1}^{(i)}), \text{ for } i = 1, \ldots, n \]
(2.23)
\[
\hat{\theta}_{n-1}^{(i)} = |S_{n-1}^{(i)}|, \text{ for } i = 1, \ldots, n \]
(2.24)
\[
\hat{\theta}_n^{(i)} = n \hat{\theta}_n - (n - 1) \hat{\theta}_{n-1}^{(i)}, \quad i = 1, \ldots, n.
\]
(2.25)
Then
\[
\hat{\theta}^*_n = n^{-1} \sum_{i=1}^{n} \hat{\theta}_n^{(i)} = \hat{\theta}_n + \frac{n-1}{n} \sum_{i=1}^{n} \hat{\theta}_n^{(i)} - \frac{n}{n-1} \hat{\theta}_{n-1}.
\]
(2.26)
Using the results in Sen (1977), it readily follows that
\[
E_F(\hat{\theta}^*_n - \theta(F)) = O(n^{-1}).
\]
(2.27)

We may consider \( \hat{\theta}^*_n \) as a competing nonparametric estimator of \( \theta(F) \).
Note that by definition

\[(n-1)S_n = (n-2)S_{n-1} + \frac{n}{n-1} (x_n - \bar{x}_n)(x_n - \bar{x}_n)'. \tag{2.28}\]

so that

\[|S_{n-1}^{(n)}| = \left| \frac{n-1}{n-2} S_n - \frac{n}{(n-1)(n-2)} (x_n - \bar{x}_n)(x_n - \bar{x}_n)' \right| \tag{2.29}\]

\[= \left( \frac{n-1}{n-2} \right) P |S_n - \frac{n}{(n-1)^2} (x_n - \bar{x}_n)(x_n - \bar{x}_n)' \right| \]

\[= \left( \frac{n-1}{n-2} \right) P |S_n | \left( 1 - \frac{n}{(n-1)^2} (x_n - \bar{x}_n)'S_n^{-1}(x_n - \bar{x}_n) \right). \]

Thus, if we define

\[a_{ni} = (x_i - \bar{x}_n)'S_n^{-1}(x_i - \bar{x}_n), \quad i = 1, \ldots, n \tag{2.30}\]

(and note that

\[\sum_{i=1}^{n} a_{ni} = \sum_{i=1}^{n} (x_i - \bar{x}_n)'S_n^{-1}(x_i - \bar{x}_n) \]

\[= \text{Tr}(S_n^{-1} \sum_{i=1}^{n} (x_i - \bar{x}_n)(x_i - \bar{x}_n)') \]

\[= (n-1)p, \]

for every \( n \geq 2 \), we obtain from (2.26) and (2.29)-(2.31) that

\[\hat{\theta}^*_n = \hat{\theta}_n - \frac{n-1}{n} \sum_{i=1}^{n} \left( \frac{n-1}{(n-1)^2} a_{ni} \right) + (n-1)\hat{\theta}_n \tag{2.32}\]

\[= \hat{\theta}_n \left( 1 - \frac{(n-1)p+1}{n(n-2)p} \right) + \sum_{i=1}^{n} \left( 1 - \frac{n}{(n-1)^2} a_{ni} \right) + n - 1 \]

\[= \hat{\theta}_n \left( 1 - \frac{(n-1)p+1}{(n-2)p} \right) + \sum_{i=1}^{n} \left( 1 - \frac{n}{n-2} \right) + n - 1 \]

\[= \hat{\theta}_n \left( 1 - \frac{(n-1)p+1}{(n-2)p} \right) \}

\[= \hat{\theta}_n \left( 1 - \frac{n}{n-2} \right) + \sum_{i=1}^{n} \left( 1 - \frac{n-1-p}{n-1} \right) \}

\[= c_{n,p} \hat{\theta}_n, \text{ say.} \]
Note that for \( p = 1, \ c_{n,1} = 1 \) while for \( p = 2, \ c_{n,p} = 1 - \frac{p-1}{2} \frac{1}{n} \cdot o(n^{-2}) \).

Thus we have

\[
|\hat{\theta}_n - \hat{\theta}| = o(n^{-1}) \quad \text{a.s., as } n \to \infty. \tag{2.33}
\]

This jackknifed estimator \((\hat{\theta}_n^*)\) belongs to the class \((\hat{\theta}_n, \hat{\theta}_n^*)\) of adjusted estimators which have been studied extensively by Sinha and others ([4], [5], [6]). It may be of interest to compare this jackknifed estimator with some of the other ones (in terms of the (asymptotic) mean squares) when \( F \) is normal. This will cast light on the (near) optimality of \( \hat{\theta}_n^* \) for normal \( F \). Details appear in Section 3.

Recall that by (2.25), (2.26) and (2.29),

\[
\hat{\theta}_{n,1} - \hat{\theta}_n^* = -n^{-1} \sum_{j=1}^{n-1} \frac{1}{n} \sum_{i=1}^{n} (\hat{\theta}_{n,i} - 1 - \frac{1}{n} \sum_{i=1}^{n} \hat{\theta}_n) \tag{2.34}
\]

\[
= -n^{-1} \sum_{j=1}^{n-1} \frac{1}{n} \sum_{i=1}^{n} (\hat{\theta}_{n,i} - 1 - \frac{1}{n} \sum_{i=1}^{n} \hat{\theta}_n) \tag{2.35}
\]

Therefore, we have

\[
\frac{1}{n-1} \sum_{i=1}^{n-1} (\hat{\theta}_{n,i} - \hat{\theta}_n) = \frac{n}{n-2} \sum_{i=1}^{n-1} (\hat{\theta}_{n,i} - \hat{\theta}_n)^2 - \frac{1}{n-1} \sum_{i=1}^{n-1} (\hat{\theta}_{n,i} - \hat{\theta}_n)^2 \tag{2.36}
\]

(2.32) and (2.35) can be used to construct an asymptotic nonparametric confidence interval for \( \theta(F) \).
3. COMPARISON WITH OPTIMAL NORMAL THEORY ESTIMATORS

When $F$ is normal, best estimators of $|\Sigma|$ of the form $c_{n,p} \hat{\theta}_n$ are known for various loss functions. For example, the optimum choice of $c_{n,p}$ is 
\[(n-p)!(n-1)p/n! = 1 + p(p-3)/2n + o(n^{-2})\] 
for each of the three losses: 
$L_1(|\hat{\Sigma}|, |\Sigma|) = (|\hat{\Sigma}| - |\Sigma|)^2$, 
$L_2(|\hat{\Sigma}|, |\Sigma|) = (|\hat{\Sigma}|/|\Sigma| - 1)^2$ and 
$L_3(|\hat{\Sigma}|, |\Sigma|) = (|\hat{\Sigma}|/|\Sigma| - \ln(|\hat{\Sigma}|/|\Sigma|) - 1$.

The risk of $c_{n,p} \hat{\theta}_n$ under $L_1(\cdot)$ is easily computed as
\[
(3.1)

\left[ (c_{n,p} - 1)^2 - c_{n,p}^2 p(p-3)/n + c_{n,p} p(p-1)/n + c_{n,p}^2 \psi_1(p)/n^2 + c_{n,p} \psi_2(p)/n^2 
+ o(n^{-2}) \right] |\Sigma|^2

\]

where $\psi_1(p)$ and $\psi_2(p)$ depend on $p$. Comparing the rises of $c_{n,p}^{opt} \hat{\theta}_n$ and $c_{n,p}^* \hat{\theta}_n$, one gets
\[
|\text{risk difference under } L_1(\cdot)| = \left[ \frac{3p^2}{n^2} + o(n^{-2}) \right] |\Sigma|^2 (3.2)
\]

The result under $L_2(\cdot)$ is obtained from (3.2) by dropping the term $|\Sigma|^2$. For the loss function $L_3(\cdot)$, the risk of $c_{n,p} \hat{\theta}_n$ is obtained as
\[
(3.3)

c_{n,p} (1 - p(p-1)/2n) - \ln c_{n,p} + c_{n,p} \psi_3(p)/n^2 + \psi_4(p,n) + o(n^{-2})
\]

where $\psi_3(p)$ depends on $p$ and $\psi_4(p,n)$ depends on both $p$ and $n$. A comparison of the risks of $c_{n,p}^{opt} \hat{\theta}_n$ and $c_{n,p}^* \hat{\theta}_n$ immediately gives
\[
|\text{risk difference under } L_3(\cdot)| = \frac{p^2}{2n^2} + o(n^{-2}). (3.4)
\]

It follows from (3.2) and (3.4) that $\hat{\theta}_n^*$ performs quite well for normal $F$ even for moderate values of $p$.

It is clear from (2.9) that the genuine nonparametric unbiased estimator $U_n$ of $\theta(F)$ is somewhat difficult for computation. However, the other competing asymptotically unbiased (up to $o(n^{-1})$) nonparametric estimator $\hat{\theta}_n^*$ is easy to work with.
4. CONCLUDING REMARKS

It is interesting to point out what happens if we consider the problem of estimation of \(|\Sigma|^{1/2} = \theta\) (say) under the nonparametric setup. First, it is clear that, unlike in the previous problem, here a kernel which can be used to construct an unbiased, symmetric, nonparametric estimator of \(\theta\) is not available. This observation automatically justifies the obvious utility of jackknifed estimators. Second, one may proceed to work with the jackknifed version of \(\hat{\theta}_n = U_n^{1/2}\) where \(U_n\) is the symmetric, unbiased estimator of \(|\Sigma|\) defined in (2.9). Various asymptotic properties of this nonparametric estimator are readily available in the form of general functions of \(U\)-statistics containing \(U_n^{1/2}\) as a special case, in Sen (1977), Section 3. Third, it is also possible to use the jackknifed version of the parametric estimator \(|S_n|^{1/2}\). Using the relations (2.29)-(2.31), it is easy to verify that this version results in \(|S_n|^{1/2}\) itself at least for large \(n\). Finally, we note that, computationally \(|S_n|^{1/2}\) much simpler than the jackknifed version of \(U_n^{1/2}\).
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