Minimum-RMS Quadratic Estimators of a Variance

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Assume that $X_1, X_2, \ldots, X_n$ are independent and identically distributed random variables with $E(X_i) = \mu$, $\mathrm{Var}(X_i) = \sigma^2$, and $E(X_i^4) < \infty$. Suppose that we are interested in estimating σ^2. Then

$$\widehat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(X_i - \mu)^2 \qquad \text{and} \qquad s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \overline{X})^2$$

both provide unbiased estimators of σ^2 where $\overline{X} = (1/n)\sum_{i=1}^{n} X_i$ is the sample mean. However, these are not generally the most efficient estimators of σ^2 in the sense of minimizing the squared error, whether the mean μ is known or unknown.

Suppose first that the X_i are normally distributed. We show below that, first,

$$S_1(\mu) = \frac{1}{n+2}\sum_{k=1}^{n}\big(X_k - \mu\big)^2 \tag{1}$$

is the estimator of the form

$$T_1(\mu) = \sum_{k=1}^{n}\sum_{\ell=1}^{n} a_{k\ell}(X_k - \mu)(X_\ell - \mu) \tag{2}$$

that minimizes $E\big(\big(T_1(\mu) - \sigma^2\big)^2\big)$ and, second, that

$$S_2 = \frac{1}{n+1}\sum_{k=1}^{n}\big(X_k - \overline{X}\big)^2 \tag{3}$$

is the estimator of the form

$$T_2 = \sum_{k=1}^{n}\sum_{\ell=1}^{n} a_{k\ell}(X_k - \overline{X})(X_\ell - \overline{X}) \tag{4}$$

that minimizes $E\big(\big(T_2 - \sigma^2\big)^2\big)$.

If the X_i are not normal, the minimum-RMS estimators become

$$S_1(\mu) = \frac{1}{n+c}\sum_{k=1}^{n}\big(X_k - \mu\big)^2 \tag{5}$$

and

$$S_2 = \frac{n}{(n+c)(n-1)+2} \sum_{k=1}^{n} (X_k - \overline{X})^2 \tag{6}$$

respectively, where

$$c \;=\; \frac{\mathrm{Var}\big((X_i-\mu)^2\big)}{\mathrm{Var}(X_i)^2} \;=\; \frac{E\big((X_i-\mu)^4\big)-\sigma^4}{\sigma^4} \tag{7}$$

Theorem. *Assume* $E(X_i) = \mu$, $\mathrm{Var}(X_i) = \sigma^2$, *and* $E(X_i^4) < \infty$ *for independent random variables* X_i. *Then*

(i) The minimum value over all symmetric matrices a_{ij} *of*

$$E\left(\left(\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(X_i-\mu)(X_j-\mu) \;-\; \sigma^2\right)^2\right) \tag{8a}$$

is attained when

$$a_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ \dfrac{1}{n+c} & \text{if } i = j \end{cases} \tag{8b}$$

for c *in (7). If the* X_i *are normal, then* $c = 2$.

(ii) The minimum value over all symmetric matrices b_{ij} *of*

$$E\left(\left(\sum_{i=1}^{n}\sum_{j=1}^{n} b_{ij}(X_i-\overline{X})(X_j-\overline{X}) \;-\; \sigma^2\right)^2\right) \tag{9a}$$

is attained when

$$b_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ \dfrac{n}{(n+c)(n-1)+2} & \text{if } i = j \end{cases} \tag{9b}$$

for c *in (7). If the* X_i *are normal, then* $b_{ii} = 1/(n+1)$.

Remark. For an alternative proof, one could begin with the fact that the expected value in (8a) is a convex function of symmetric matrices a (and that it also satisfies the parallelogram law) and conclude that any minimal solution of (8a) or (9a) must be of the form

$$a_{ij} \;=\; \begin{cases} a & \text{if } i = j \\ b & \text{if } i \neq j \end{cases}$$

However, this only helps slightly in the proof of part (i) and seems to make the proof of (ii) more difficult. See later remarks for more details.

Proof of Theorem. (i) Assume $E(X_i) = \mu = 0$ and consider

$$\phi(a) \;=\; E\left(\left(\sum_{k=1}^{n}\sum_{\ell=1}^{n} a_{k\ell}X_kX_\ell \;-\; \sigma^2\right)^2\right) \tag{10a}$$

as a function of $n(n+1)/2$ variables a_{ij} $(1 \le i \le j \le n)$. Then

$$\begin{aligned}\frac{\partial}{\partial a_{ij}}\,\phi(a) \;&=\; C_{ij}\,E\left(X_iX_j\left(\sum_{k=1}^{n}\sum_{\ell=1}^{n} a_{k\ell}X_kX_\ell \;-\; \sigma^2\right)\right)\\ &=\; C_{ij}\left(\sum_{k=1}^{n}\sum_{\ell=1}^{n} a_{k\ell}E(X_iX_jX_kX_\ell) \;-\; \sigma^2 E(X_iX_j)\right)\end{aligned} \tag{10b}$$

where $C_{ij} = 4$ if $i \ne j$ and $C_{ij} = 2$ if $i = j$. Since the X_i are independent and $E(X_i) = 0$, $E(X_iX_j) = E(X_i)E(X_j) = 0$ if $i \ne j$ and $E(X_aX_bX_cX_d) = 0$ if any of the indices a, b, c, d are unmatched. This leads to

$$\frac{\partial}{\partial a_{ij}}\,\phi(a) \;=\; \begin{cases} 8a_{ij}\sigma^4 & \text{if } i \ne j \\ 2\left(\sum_{k=1}^{n} a_{kk}E(X_k^2X_i^2) - \sigma^4\right) & \text{if } i = j \end{cases} \tag{10c}$$

The first equation above implies $a_{ij} = 0$ if $i \ne j$ at a minimum value of (10a). The second equation implies

$$a_{ii}\left(E(X_i^4) - E(X_i^2)^2\right) \;+\; \left(\sum_{k=1}^{n} a_{kk}\right)\sigma^4 - \sigma^4 \;=\; 0$$

for $1 \le i \le n$. Thus $a_{ii} = a$ where $a\,\mathrm{Var}(X_i^2) + na\sigma^4 = \sigma^4$ so that $a_{ii} = a = \sigma^4/\big(\mathrm{Var}(X_i^2) + n\sigma^4\big) = 1/(n+c)$ for $c = \mathrm{Var}(X_i)/\sigma^4$. This implies (8b), which is the first part of the theorem. If the X_i are normal with mean zero, then $E(X_i^4) = 3\sigma^4$ and $c = 2$.

(ii) If $\overline{c}_{i+} = (1/n)\sum_{j=1}^{n} c_{ij}$ for a general matrix c_{ij}, then

$$\sum_i\sum_j b_{ij}\overline{c}_{i+} = \frac{1}{n}\sum_i\sum_j\sum_k b_{ij}c_{ik} = \sum_i\sum_j(\overline{b}_{i+})c_{ij}$$

It follows that

$$\sum_{i=1}^{n}\sum_{j=1}^{n} b_{ij}(X_i - \overline{X})(X_j - \overline{X}) \;=\; \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(X_i - d)(X_j - d) \tag{11a}$$

for any constant d where

$$a_{ij} = b_{ij} - \overline{b}_{i+} - \overline{b}_{+j} + \overline{b}, \qquad \overline{b} = \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} b_{ij} \tag{11b}$$

An arbitrary symmetric matrix a_{ij} can be written in the form (11b) for some other matrix b_{ij} if and only if $\overline{a}_{i+} = 0$ for $1 \le i \le n$. Thus if $E(X_i) = d = 0$

$$\min_b E\left(\left(\sum_{i=1}^{n}\sum_{j=1}^{n} b_{ij}(X_i - \overline{X})(X_j - \overline{X}) \;-\; \sigma^2\right)^2\right) \tag{12a}$$

$$= \;\min_a E\left(\left(\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}X_iX_j \;-\; \sigma^4\right)^2\right) \tag{12b}$$

subject to the conditions $\overline{a}_{i+} = 0$ for $1 \le i \le n$.

We use Lagrange multipliers in (12b) with the n constaints $\psi_p(a) = \sum_{k=1}^{n} a_{pk} = 0$ $(1 \le p \le n)$ for symmetric matrices a. This leads to

$$\frac{\partial}{\partial a_{ij}}\left(\phi(a) - \sum_{p=1}^{n}\lambda_p\psi_p(a)\right) \;=\; 0$$

for $1 \le i \le j \le n$, $\phi(a)$ in (10a), and n additional constants λ_p. The relations (10c) imply

$$8a_{ij}\,\sigma^4 - \lambda_i - \lambda_j = 0, \qquad i \ne j \tag{13a}$$

$$2a_{ii}\left(E(X_i^4) - \sigma^4\right) + 2\left(\sum_{k=1}^{n} a_{kk}\right)\sigma^4 - 2\sigma^4 - \lambda_i = 0, \quad i = j \tag{13b}$$

Set $\theta = E(X_i^4) - \sigma^4$ and $\Lambda = \sum_{k=1}^{n}\lambda_k$. Since $\sum_{j=1}^{n} a_{ij} = 0$, we must have $\sum_{j=1, j\ne i}^{n} a_{ij} = -a_{ii}$. Applying this in (13) implies $-8a_{ii}\sigma^4 - (n-1)\lambda_i - (\Lambda - \lambda_i) = 0$ and

$$a_{ii}8\sigma^4 + (n-2)\lambda_i = -\Lambda \tag{14a}$$

$$a_{ii}2\theta - \lambda_i = 2\sigma^4\left(1 - \sum_{k=1}^{n} a_{kk}\right) \tag{14b}$$

The negative of the determinant of the 2×2 system (14) for a_{ii} and λ_i is $8\sigma^4 + 2\theta(n-2) > 0$ since $\theta \geq 0$, excluding the trivial case $\sigma^2 = 0$. This means that $a_{ii} = a$ and $\lambda_i = \lambda$ are both constant. In particular $\Lambda = n\lambda$ and (14) simplifies to

$$\begin{aligned} a8\sigma^4 + (2n-2)\lambda &= 0 \\ a2\theta - \lambda &= 2\sigma^4(1-na) \end{aligned} \tag{15}$$

Thus $\lambda = -4a\sigma^4/(n-1)$ and

$$\begin{aligned} 2a\left(\theta + \frac{2\sigma^4}{n-1} + n\sigma^4\right) &= 2\sigma^4 \\ a = a_{ii} &= \frac{n-1}{(n+c)(n-1)+2} \end{aligned} \tag{16}$$

since $\theta/\sigma^4 = c$. It follows from (13a) that $a_{ij} = 2\lambda/(8\sigma^4) = -a/(n-1)$ if $i \neq j$, which also follows from $\sum_{j=1}^n a_{ij} = 0$.

Finally, the quadratic form in b_{ij} in (11a) is the same if you add any constant to all of its entries. Thus there is a diagonal matrix $b_{ij} = a_{ij} + a/(n-1)$ that minimizes (12a) with

$$b_{ii} = a_{ii} + \frac{a}{n-1} \;=\; a\frac{n}{n-1} \;=\; \frac{n}{(n+c)(n-1)+2}$$

If the X_i are normal, then $c = 2$ and $b_{ii} = 1/(n+1)$, which completes the proof of the theorem.

An Alternative Approach. The function

$$\phi(a) \;=\; E\left(\left(\sum_{k=1}^n\sum_{\ell=1}^n a_{k\ell}X_kX_\ell \;-\; \sigma^2\right)^2\right) \tag{10}$$

is a convex function of symmetric matrices a viewed as points in $R^{n(n+1)/2}$. We also have the "parallelogram identity"

$$\frac{\phi(a)+\phi(b)}{2} \;=\; \phi\left(\frac{a+b}{2}\right) \;+\; \phi\left(\frac{a-b}{2}\right) \tag{11}$$

Now suppose that a is the minimum value of (10). Since the X_i are identically distributed, $\phi(b) = \phi(a)$ whenever $b = P'aP$ and P is any permutation of the coordinates. In that case, $b_{ij} = a_{\pi_i\pi_j}$, where π is a permutation of

$\{1, 2, 3, \ldots, n\}$. Thus if $\phi(a)$ is the minimum value of (10), then $\phi(a) = \phi(b)$ whenever $b = P'aP$, and $\phi((a+b)/2)$ must also be the minimum. This implies $\phi((a-b)/2) = 0$ and

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_{ij} X_i X_j \;=\; 0 \quad \text{almost surely for} \quad c = (a-b)/2$$

We can conclude from this that $c = 0$ unless the X_i are highly singular and thus $a = b = P'aP$. If $a = P'aP$ for all permutation matrices P, then

$$a_{ij} \;=\; \begin{cases} a & \text{if } i = j \\ b & \text{if } i \neq j \end{cases}$$

for constants a and b. However, this turns out not to simply the proofs of parts (i) and (ii) of the theorem a great deal, and actually seems to make the proof of part (ii) more difficult.