Unbiased estimation of fourth-order matrix moments

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ABSTRACT

We formulate Browne's (1984) unbiased estimator for the elements of the matrix of fourth-order moments in terms of matrices. We show that this matrix is indeed an unbiased estimator, without using the theory of cumulants and k-statistics.

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*Comments by Caroline Couperus and an anonymous referee are gratefully acknowledged. The usual disclaimer applies.

655 Avenue of the Americas, New York, NY 10010 0024-3795/92/$3.50

1. INTRODUCTION

Suppose we have n independent realizations $x_1, \ldots, x_n$ of a random $p \times 1$ vector x, which has a distribution with mean $\mu \equiv \mathscr{E}(x)$, variance $K \equiv \mathscr{D}(x)$, fourth-order moment $\mathbf{W} \equiv \mathscr{E}[(x-\mu)(x-\mu)' \otimes (x-\mu)(x-\mu)']$, and finite eighth-order moment. The usual unbiased estimator for K is

$$\hat{K} \equiv \frac{1}{n-1} X'NX,$$

where $X' \equiv (x_1, \ldots, x_n)$ and $N \equiv I - (1/n)\, \iota\iota'$, ι being an $n \times 1$ vector of ones. The matrix N transforms observations into deviations from their means. Let $\hat{k} \equiv \operatorname{vec} \hat{K}$, and let $\mathscr{D}(\hat{k})$ be the population variance of $\hat{k}$. How can one find an unbiased estimator $\hat{D}$ of $\mathscr{D}(\hat{k})$?

Browne (1984) gave the answer, using certain results on scalar cumulants and k-statistics. In this paper we reformulate Browne's estimator in matrix form and show that it is an unbiased estimator of $\mathscr{D}(\hat{k})$. Our proof of unbiasedness is direct and is not based on the theory of cumulants and k-statistics.

The paper is organized as follows. In Section 2 we present a useful operator and some matrix notation. In Section 3 we present Browne's estimator in matrix form. In Section 4 we derive an auxiliary result that we use in Section 5 to prove the unbiasedness of Browne's estimator. In the final section we discuss our results in relation to the theory of cumulants.

2. THE TILDE OPERATOR

The first thing to do is to define a special operator, which we will call the *tilde operator*. This operator transforms a matrix of order $m^2 \times m^2$, say,

$$A = \begin{pmatrix} A_{11} & \cdots & A_{1m} \\ \vdots & & \vdots \\ A_{m1} & \cdots & A_{mm} \end{pmatrix} = \sum_{i,j} (E_{ij} \otimes A_{ij}),$$

whose submatrices are square of order m, into

$$\tilde{A} = (\text{vec}\, A_{11}, \ldots, \text{vec}\, A_{m1}, \ldots, \text{vec}\, A_{mm}) = \sum_{i,j} (\text{vec}\, A_{ij})(\text{vec}\, E_{ij})',$$

where $E_{ij} \equiv e_i e_j'$ and e_i is the ith unit vector of order $m \times 1$. It is easy to see that

$$\text{vec}\, \tilde{A} = \sum_{i,j} (\text{vec}\, E_{ij} \otimes \text{vec}\, A_{ij}) = (I_m \otimes P_{mm} \otimes I_m)\, \text{vec}\, A,$$

where P_{mm} is the commutation matrix (see Magnus and Neudecker 1979, Wansbeek 1989). We used Theorem 3.1(i) of Neudecker and Wansbeek (1983) to take the second step. Both the commutation matrix P and the tilde operator can be generalized to apply to matrices with a less specific structure than A, but for our purpose there is no need to do so.

If D and F are square $m \times m$ matrices and C is partitioned into square $m \times m$ blocks, we are able to prove the following results, which we will use in the sequel:

$$\text{if} \quad C = D \otimes F \quad \text{then} \quad \tilde{C} = (\text{vec}\, F)(\text{vec}\, D)'; \tag{2.1}$$

$$\text{if} \quad C = (\text{vec}\, F)(\text{vec}\, D)' \quad \text{then} \quad \tilde{C} = D \otimes F; \tag{2.2}$$

$$\text{if} \quad C = P_{mm}(D \otimes F) \quad \text{then} \quad \tilde{C} = P_{mm}(D \otimes F'). \tag{2.3}$$

For more properties of the tilde operator and generalizations, we refer to Koning, Neudecker, and Wansbeek (1990).

Proof of (2.1). $\text{vec}\tilde{C} = (I_m \otimes P_{mm} \otimes I_m)\text{vec}C = (I_m \otimes P_{mm} \otimes I_m)(I_m \otimes P_{mm} \otimes I_m)$ $(\text{vec}\, D \otimes \text{vec}\, F) = \text{vec}\{(\text{vec}\, F)(\text{vec}\, D)'\}$. As $\tilde{C}$ and $(\text{vec}\, F)(\text{vec}\, D)'$ are matrices of the same order, we conclude that $\tilde{C} = (\text{vec}\, F)(\text{vec}\, D)'$. *Mutatis mutandis*, this reasoning applies to the following proofs as well. ■

Proof of (2.2). $\text{vec}\, \tilde{C} = (I_m \otimes P_{mm} \otimes I_m)\, \text{vec}\, C = (I_m \otimes P_{mm} \otimes I_m)$ $\text{vec}\{(\text{vec}\, F)(\text{vec}\, D)'\} = (I_m \otimes P_{mm} \otimes I_m)(\text{vec}\, D \otimes \text{vec}\, F) = \text{vec}(D \otimes F)$. ■

Proof of (2.3). $\operatorname{vec}\tilde{C} = (I_m \otimes P_{mm} \otimes I_m)\operatorname{vec}\{P_{mm}(D \otimes F)\} = (I_m \otimes P_{mm} \otimes I_m)$ $\operatorname{vec}\{(F \otimes D)P_{mm}\} = \operatorname{vec}\{(F' \otimes D)P_{mm}\} = \operatorname{vec}\{P_{mm}(D \otimes F')\}$, using Lemma 4.1(i) of Neudecker and Wansbeek (1983). ■

Let $y \equiv x - \mu$. In Section 4, we use two properties of the matrix of fourth-order moments $\mathbf{W} \equiv \mathscr{E}(yy' \otimes yy')$, viz.

$$\tilde{\mathbf{W}} = \mathbf{W} \tag{2.4}$$

and

$$P_{mm}\mathbf{W} = \mathbf{W}. \tag{2.5}$$

These results are straightforwardly proven:

$$\begin{aligned}\tilde{\mathbf{W}} &= \mathscr{E}(yy' \tilde{\otimes} yy') = \mathscr{E}\{\operatorname{vec}(yy')\}\{\operatorname{vec}(yy')\}' \\ &= \mathscr{E}(y \otimes y)(y \otimes y)' = \mathscr{E}(yy' \otimes yy') = \mathbf{W},\end{aligned}$$

by applying (2.1) in the first step; and

$$\begin{aligned}P_{mm}\mathbf{W} &= \mathscr{E}\{P_{mm}[yy' \otimes yy']\} \\ &= \mathscr{E}\{P_{mm}(y \otimes y)(y \otimes y)'\} = \mathscr{E}(y \otimes y)(y \otimes y)' = \mathbf{W},\end{aligned}$$

as $P_{mm}(y \otimes y) = P_{mm}\operatorname{vec}(yy') = \operatorname{vec}(yy')$, yy' being a symmetric matrix.

3. BROWNE'S ESTIMATOR

From now on we make a useful simplification: we will consider the $p \times 1$ vector $y \equiv x - \mu$ rather than x. Since all expressions in X that we employ are of the form NX, and because $NX = NY$, with

$$Y' \equiv (y_1, \ldots, y_n) = (x_1 - \mu, \ldots, x_n - \mu).$$

this simplification is without loss of generality.

Browne's results are that

$$d_{ijkl} \equiv \frac{n(n-1)}{(n-2)(n-3)}\left\{w_{ijkl} - \left(\frac{n-1}{n}\right)^2 k_{ij}k_{kl}\right\}$$

$$-\frac{(n-1)^2}{n(n-2)(n-3)}\left\{k_{ik}k_{jl} + k_{il}k_{jk} - \frac{2}{n-1}k_{ij}k_{kl}\right\}$$

is an unbiased estimator for $\operatorname{cov}\left\{(n-1)^{1/2}k_{ij}, (n-1)^{1/2}k_{kl}\right\}$, and the latter is

$$\frac{n-1}{n}\sigma_{ijkl} + \frac{1}{n}(\kappa_{ik}\kappa_{jl} + \kappa_{il}\kappa_{jk}) - \frac{n-1}{n}\kappa_{ij}\kappa_{kl}.$$

In these formulas, $w_{ijkl} = (1/n)\Sigma_\alpha(y_{i\alpha} - \bar{y}_i)(y_{j\alpha} - \bar{y}_j)(y_{k\alpha} - \bar{y}_k)(y_{l\alpha} - \bar{y}_l)$, where the indices i, j, k, and l refer to elements of y; k_{ij} is the (i,j)th element of $\hat{K}$; κ_{ij} is the (i,j)th element of K; and $\sigma_{ijkl} = \mathscr{E}(y_i y_j y_k y_l)$.

Let

$$\hat{\mathrm{W}} \equiv \frac{1}{n}(Y\otimes Y)'(N\otimes N)\Delta(N\otimes N)(Y\otimes Y),$$

be an estimator for W, with $\Delta \equiv \Sigma_k(E_{kk}\otimes E_{kk})$. Now we have that, in matrix notation,

$$\hat{D} = \frac{n-1}{n(n-2)(n-3)}\left(\frac{n^2}{n-1}\hat{\mathrm{W}} - (I+P)(\hat{K}\otimes\hat{K}) - \hat{k}\hat{k}'\right) - \frac{1}{n-2}\hat{k}\hat{k}' \quad (3.1)$$

is an unbiased estimator for $\mathscr{D}(\hat{k})$. The latter quantity is

$$\mathscr{D}(\hat{k}) = \frac{1}{n}\mathrm{W} + \frac{1}{n(n-1)}(I+P)(K\otimes K) - \frac{1}{n}kk'. \quad (3.2)$$

Note that we do not scale $\hat{k}$ by $(n-1)^{1/2}$ as is done by Browne. We will now prove (3.2) and the unbiasedness of (3.1).

4. AN AUXILIARY RESULT AND SOME APPLICATIONS

The starting point in our analysis is the following expectation:

$$\begin{aligned}\mathscr{E}(Y'RY\otimes Y'RY) &= \mathscr{E}\Big(\sum_{i,j} r_{ij}y_iy_j'\otimes \sum_{k,l} r_{kl}y_ky_l'\Big)\\ &= \mathscr{E}\Big\{\sum_i r_{ii}^2 y_iy_i'\otimes y_iy_i'\\ &\quad + \sum_{i\neq j}\big(r_{ii}r_{jj}y_iy_i'\otimes y_jy_j' + r_{ij}^2 y_iy_j'\otimes y_iy_j' + r_{ij}^2 y_iy_j'\otimes y_jy_i'\big)\Big\}\\ &= \sum_i r_{ii}^2 W + \sum_{i\neq j}\{r_{ii}r_{jj}K\otimes K + r_{ij}^2 kk' + r_{ij}^2 P(K\otimes K)\},\end{aligned} \tag{4.1}$$

where $R = (r_{ij})$ is a symmetric matrix. Note that the second equality is based on the omission of all terms in the fourfold summation preceding it that contain y's with a unique index. These terms have expectation zero.

There are two applications of this result. First, for $R = N = (n_{ij})$ there follows immediately

$$\begin{aligned}\mathscr{E}(\hat{K}\otimes\hat{K}) &= \frac{1}{(n-1)^2}\mathscr{E}(Y'NY\otimes Y'NY)\\ &= \frac{1}{(n-1)^2}\Big(\frac{(n-1)^2}{n}W + \frac{(n-1)^3}{n}K\otimes K\\ &\qquad + \frac{n-1}{n}[P(K\otimes K) + kk']\Big)\\ &= \frac{1}{n}W + \frac{n-1}{n}K\otimes K + \frac{1}{n(n-1)}\{P(K\otimes K) + kk'\},\end{aligned} \tag{4.2}$$

since $r_{ii} = n_{ii} = 1 - 1/n$ and $r_{ij} = n_{ij} = -1/n$ $(i \neq j)$. On premultiplying the left-hand and right-hand sides of (4.2) by P, we find

$$\mathscr{E}[P(\hat{K}\otimes\hat{K})] = \frac{1}{n}W + \frac{n-1}{n}P(K\otimes K) + \frac{1}{n(n-1)}\{K\otimes K + kk'\}. \tag{4.3}$$

using (2.5), and on applying the tilde operator to (4.2), we obtain

$$\mathscr{E}(\hat{k}\hat{k}') = \frac{1}{n}\mathbf{W} + \frac{1}{n(n-1)}(I+P)(K\otimes K) + \frac{n-1}{n}kk', \qquad (4.4)$$

using (2.4). As a corollary to the latter,

$$\mathscr{D}(\hat{k}) = \mathscr{E}(\hat{k}\hat{k}') - kk' = \frac{1}{n}\mathbf{W} + \frac{1}{n(n-1)}(I+P)(K\otimes K) - \frac{1}{n}kk'. \quad (4.5)$$

This expression was also given by Traat (1984, Equation (15)). This proves (3.2).

The other application of (4.1) is to evaluate $\mathscr{E}(\hat{\mathbf{W}})$. Since

$$\hat{\mathbf{W}} = \frac{1}{n}\sum_k (Y'NE_{kk}NY \otimes Y'NE_{kk}NY),$$

and $E_{kk} = e_k e_k$, we have to evaluate first

$$Ne_k = \left(I - \frac{1}{n}\iota\iota'\right)e_k = e_k - \frac{1}{n}\iota,$$

$$e_k' N e_l = \delta_{kl} - \frac{1}{n},$$

where δ_{kl} is Kronecker's delta, so for this case

$$\sum_i r_{ii}^2 = \sum_i \left(\delta_{ij} - \frac{1}{n}\right)^4 = \left(1 - \frac{1}{n}\right)^4 + \frac{n-1}{n^4}$$

$$= \frac{(n-1)(n^2-3n+3)}{n^3},$$

$$\sum_{i\neq j} r_{ii}r_{jj} = \sum_{i\neq j} r_{ij}^2 = \sum_{i\neq j}\left(\delta_{kl} - \frac{1}{n}\right)^2\left(\delta_{jk} - \frac{1}{n}\right)^2$$

$$= \frac{(n-1)(2n-3)}{n^3}.$$

Insertion of these summations in (4.1) yields

$$\mathscr{E}(\hat{W}) = \frac{n-1}{n^3}\{(n^2-3n+3)W+(2n-3)[(I+P)(K\otimes K)+kk']\}. \quad (4.6)$$

5. PROOF OF UNBIASEDNESS

We can collect the equations (4.2), (4.3), (4.4), and (4.6) as follows:

$$\mathscr{E}\begin{pmatrix} \hat{K}\otimes\hat{K} \\ P(\hat{K}\otimes\hat{K}) \\ \hat{k}\hat{k}' \\ \hat{W} \end{pmatrix} = \frac{1}{n(n-1)}$$

$$\times\left\{\begin{bmatrix} (n-1)^2 & 1 & 1 & n-1 \\ 1 & (n-1)^2 & 1 & n-1 \\ 1 & 1 & (n-1)^2 & n-1 \\ a & a & a & b \end{bmatrix}\otimes I\right\}$$

$$\times\begin{pmatrix} K\otimes K \\ P(K\otimes K) \\ kk' \\ W \end{pmatrix}, \quad (5.1)$$

where

$$a \equiv \left(\frac{n-1}{n}\right)^2(2n-3) \quad \text{and} \quad b \equiv \left(\frac{n-1}{n}\right)^2(n^2-3n+3).$$

We can also rewrite (4.5) in this format and reformulate our task into that of finding an unbiased estimator of

$$\mathscr{D}(\hat{k}) = \frac{1}{n(n-1)}\{(1,1,1-n,n-1)\otimes I\}\begin{pmatrix} K\otimes K \\ P(K\otimes K) \\ kk' \\ W \end{pmatrix}. \quad (4.5')$$

In condensed form, we can write (5.1) and (4.5′) as

$$\mathscr{E}(\hat{T}) = \frac{1}{n(n-1)}(M \otimes I)T,$$

$$\mathscr{D}(\hat{k}) = \frac{1}{n(n-1)}(g' \otimes I)T,$$

with M, g, $\hat{T}$, and T implicitly defined. So

$$\hat{D} = (g'M^{-1} \otimes I)\hat{T} \tag{5.2}$$

is by construction an unbiased estimator of $\mathscr{D}(\hat{k})$. It remains to evaluate $g'M^{-1}$. It can be given in the following form:

$$h' \equiv g'M^{-1} = \left(-c, -c, -c - \frac{1}{n-2}, \frac{n^2}{n-1}c\right), \tag{5.3}$$

with $c \equiv (n-1)/n(n-2)(n-3)$. This can be shown by straightforward multiplication, by verifying $h'M = g'$. An auxiliary result is

$$\begin{aligned}
&\left(-1, -1, -1, \frac{n^2}{n-1}\right)\begin{pmatrix}(n-1)^2\\ 1\\ 1\\ a\end{pmatrix}\\
&\quad = \left(\frac{n^2}{n-1}\right)\left(\frac{n-1}{n}\right)^2(2n-3) - 2 - (n-1)^2\\
&\quad = (n-1)(2n-3) - 2 - (n-1)^2\\
&\quad = n^2 - 3n = n(n-3),
\end{aligned}$$

so the first two elements of $h'M$ obey

$$h'Me_1 = h'Me_2 = cn(n-3) - \frac{1}{n-2} = 1 = g'e_2 = g'e_1,$$

and the third obeys

$$h'Me_3 = cn(n-3) - \frac{1}{n-2}(n-1)^2 = 1 - n = g'e_3.$$

Finally, for the fourth element, we have

$$h'Me_4 = c\left[\left(\frac{n^2}{n-1}\right)\left(\frac{n-1}{n}\right)^2(n^2-3n+3) - 3(n-1)\right] - \frac{n-1}{n-2}$$

$$= cn(n-1)(n-3) - \frac{n-1}{n-2} = n - 1 = g'e_4.$$

Hence $h'M = g'$, and a comparison of (5.2) and (5.3) with (3.1) shows that the latter indeed presents an unbiased estimator of $\mathscr{D}(\hat{k})$. Of course, we can derive unbiased estimators for all linear combinations of the elements of T, using this procedure.

6. MULTIVARIATE CUMULANTS

Browne derived his result by using scalar results on multivariate cumulants. This section shows the connection between the theory of cumulants and our results.

First, note that the matrix K has elements κ_{ij}, the second-order cumulants of y. The matrix $\mathbf{K}$ is the matrix with elements κ_{ijkl}, the fourth-order cumulants of y:

$$\mathbf{K} \equiv \mathbf{W} - (I + P)(K \otimes K) - kk'. \tag{6.1}$$

This expression was also given by Traat (1984, Equation (16)). Further we define

$$\hat{\mathbf{K}} \equiv \frac{n^2(n+1)}{(n-1)(n-2)(n-3)}\hat{\mathbf{W}} - \frac{(n-1)^2}{(n-2)(n-3)}\left\{(I+P)(\hat{K}\otimes\hat{K}) + \hat{k}\hat{k}'\right\}. \tag{6.2}$$

The matrices $\hat{\mathbb{K}}$ and $\hat{K}$ have elements k_{ijkl} and k_{ij}, the so-called k-statistics. The k-statistics are unbiased estimators for the corresponding cumulants (see for instance Kaplan 1952), and hence, $\hat{K}$ and $\hat{\mathbb{K}}$ are unbiased estimators for K and $\mathbb{K}$. A proof of the latter case in matrix format can be given analogously to the proof of the unbiasedness of $\hat{D}$:

$$\mathbb{K} = (r' \otimes I)T$$

and

$$\hat{\mathbb{K}} = (q' \otimes I)\hat{T},$$

where $r' \equiv (-1, -1, -1, 1)$ and

$$q' \equiv \left(-d, -d, -d, \frac{n^2(n+1)}{(n-1)^3} d \right), \qquad \text{with} \quad d \equiv \frac{(n-1)^2}{(n-2)(n-3)}.$$

It is easily verified that $q'M = r'$, and hence that $\mathscr{E}(\hat{\mathbb{K}}) = \mathbb{K}$. By insertion of (6.1) in (3.2) we can express $\mathscr{D}(\hat{k})$ in terms of cumulants:

$$\mathscr{D}(\hat{k}) = \frac{1}{n}\mathbb{K} + \frac{1}{n-1}(I+P)(K \otimes K) \tag{6.3}$$

(also given by Traat, 1984), and if we insert (6.2) in (3.1) we obtain

$$\hat{D} = \frac{n-1}{n(n+1)}\hat{\mathbb{K}} + \frac{n-1}{(n-2)(n+1)}(I+P)(\hat{K} \otimes \hat{K}) - \frac{2}{(n-2)(n+1)}\hat{k}\hat{k}'$$

as an expression for $\hat{D}$ in terms of k-statistics.

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Received 27 March 1990; final manuscript accepted 24 October 1990

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