Distribution of random quadratic forms arising in singular-spectrum analysis

VALENTINA G. MOSKVINA*

Abstract. *We derive explicit expressions for the coefficients of certain quadratic forms arising in the singular-spectrum analysis, a novel technique of time series analysis. We also derive expressions for the first two moments of these quadratic forms under the assumption that the time series is a sum of a linear trend and white noise.*

Key words: *time series analysis, random quadratic forms, singular-spectrum analysis, trajectory matrix, centring*

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1. Introduction

One of the methods of time series analysis, that has recently attracted a lot of attention, is the so-called singular-spectrum analysis (SSA), see Elsher and Tsonis (1996) for an introduction and Golyandina, Nekrutkin and Zhigljavsky (2001) for a detailed description of the methodology and theory.

Let $y_1, y_2, \ldots$ be a time series. SSA is based on the singular-value decomposition of the so-called "trajectory matrix"

$$\mathbf{X} = (x_{ij})_{ij=1}^{M,K} = \begin{pmatrix} y_1 & y_2 & y_3 & \cdots & y_K \\ y_2 & y_3 & y_4 & \cdots & y_{K+1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y_M & y_{M+1} & y_{M+2} & \cdots & y_N \end{pmatrix} \tag{1}$$

where N is the number of observations, M is an integer called "lag parameter" $(M \leq N/2)$, $K = N - M + 1$ and $x_{ij} = y_{i+j-1}$ for all $i = 1 \ldots, M$, $j = 1 \ldots, K$.

In many cases performing a singe or double centring of the trajectory matrix is recommended, see Golyandina, Nekrutkin and Zhigljavsky (2001). Denote by $\mathbf{Z}$ the matrix obtained from $\mathbf{X}$ after a centring operation is performed.

Single centring means that the row averages are subtracted from each element of the matrix $\mathbf{X}$; that is, the elements of $\mathbf{Z}$ are

$$z_{ij} = x_{ij} - \frac{1}{M} \sum_{i=1}^{M} x_{ij} \,. \tag{2}$$

*School of Mathematics, Cardiff University, P.O. Box 926, Cardiff CF24 4YH, United Kingdom, e-mail: `MoskvinaV@Cardiff.ac.uk`

If we subtract the row and column averages from x_{ij} and add the general mean, then we obtain double centring of the trajectory matrix. The resulted $M\times K$-matrix $\mathbf{Z}=(z_{ij})_{ij=1}^{M,K}$ has the elements

$$z_{ij}=x_{ij}-\frac{1}{M}\sum_{i=1}^{M}x_{ij}-\frac{1}{K}\sum_{j=1}^{K}x_{ij}+\frac{1}{MK}\sum_{i=1}^{M}\sum_{j=1}^{K}x_{ij}\,. \tag{3}$$

Obviously, we could use the formulae (2) and (3) to compute the values z_{ij} for $j>K$; this corresponds to the use of y_t with $t>N$.

The following sum of squares

$$SS_{p,q}=\sum_{i=1}^{M}\sum_{j=p+1}^{q}z_{ij}^2 \tag{4}$$

is of high importance in the theory of SSA in relation to the problems of detection of structural heterogeneities in time series, see Chapter 3 in Golyandina, Nekrutkin and Zhigljavsky (2001), Moskvina and Zhigljavsky (2000) and the Website http://www.cf.ac.uk/maths/stats/changepoint/ . Here p and q are arbitrary integers, $0\le p<q$.

The case when $p=0$ and $q=K$ is of a particular interest. Another important case is when $p\ge K$; in this case the sum of squares is computed for the subseries that contain points lying outside the interval $[1,N]$.

We will demonstrate that the sum of squares $SS_{p,q}$ can be represented as a quadratic form

$$SS_{p,q}=e^TBe, \tag{5}$$

where $e=(e_1,\ldots,e_{q+M-1})^T$ is some vector that can often be associated with the observation noise in the original series $y_1,y_2,\ldots$ and B is a $(q+M-1)\times(q+M-1)$ matrix.

In *Section 2* we consider the most difficult case of double centring. We assume that $y_t=a+bt+e_t\quad(t=1,2,\ldots)$, where a and b are unknown parameters and e_t is noise.

If b is known (and we thus can assume $b=0$), then there is no need to do double centring of the trajectory matrix X to achieve independence of a, the subtraction of the row averages would suffice. This case is considered in *Section 3*.

In the simplest case, when both a and b are known (we thus can assume $a=b=0$), we do not need to do centring at all to achieve independence of a and b. We thus have $z_{ij}=x_{ij}=y_{i+j-1}$ in the formula for $SS_{p,q}$; the case of no centring is considered in *Section 4*.

In all three cases we shall compute the matrix B and the first two moments under the assumption that e_t are independent normal random variables with $Ee_t=0$ and $\mathrm{var}(e_t)=\sigma^2=const$.

To compute the moments, we will use the results on distributions of quadratic forms of random variables, see e.g. Section 3.2 in Mathai and Provost (1992) and Section 2.5 in Searle (1971). These results imply that

$$E(e^TBe)=\sigma^2\mathrm{tr}B\,, \tag{6}$$

$$\mathrm{var}(e^T Be) = 2\sigma^4 \mathrm{tr} B^2 \tag{7}$$

Note that the proof of (6) does not require normality of e_t and that both properties (6) and (7) can be easily generalized to the case when the components of e are dependent (e.g. to the case when e_t is an autoregressive process).

2. Double centring

2.1. Notation

Assume that $y_t = a+bt+e_t \quad (t = 1, 2, \ldots)$, where a and b are unknown parameters and e_t is noise. Consider the case of double centring, when the elements of the matrix $\mathbf{Z}$ are defined by (3).

An important observation about the matrix $\mathbf{Z}$ is that its elements z_{ij} do not depend on the actual values of the parameters a and b. Indeed, we can write $x_{ij} = a+b(i+j-1)+\varepsilon_{ij}$, where $\varepsilon_{ij} = e_{i+j-1}$, and therefore we obtain

$$\begin{aligned} z_{ij} &= a + b(i+j-1) + \varepsilon_{ij} + \frac{1}{KM}\sum_{i=1}^{M}\sum_{j=1}^{K}(a + b(i+j-1) + \varepsilon_{ij}) \\ &\quad -\frac{1}{M}\sum_{i=1}^{M}(a + b(i+j-1) + \varepsilon_{ij}) - \frac{1}{K}\sum_{j=1}^{K}(a + b(i+j-1) + \varepsilon_{ij}) \\ &= \varepsilon_{ij} - \varepsilon_{.j} - \varepsilon_{i.} + \varepsilon_{..}\,, \end{aligned}$$

where

$$\varepsilon_{i.} = \frac{1}{K}\sum_{k=1}^{K}\varepsilon_{ik}, \quad \varepsilon_{.j} = \frac{1}{M}\sum_{i=1}^{M}\varepsilon_{ij}, \quad \varepsilon_{..} = \frac{1}{MK}\sum_{i=1}^{M}\sum_{k=1}^{K}\varepsilon_{ik} \tag{8}$$

Denote $Q = q-p$. To formulate the results, we shall need the function $w_{M,p,q}(t)$ which is defined as follows (see also *Figure 1*):
if $M \le Q$,

$$w_{M,p,q}(t) = \begin{cases} t-p, & \text{for } p < t \le p+M \\ M, & \text{for } p+M < t \le q \\ q+M-t, & \text{for } q < t \le q+M \\ 0, & \text{otherwise} \end{cases} \tag{9}$$

and, if $0 < Q \le M$,

$$w_{M,p,q}(t) = \begin{cases} t-p, & \text{for } p < t \le q \\ Q, & \text{for } q < t \le M+p \\ q+M-t, & \text{for } M+p < t \le M+q \\ 0, & \text{otherwise.} \end{cases} \tag{10}$$

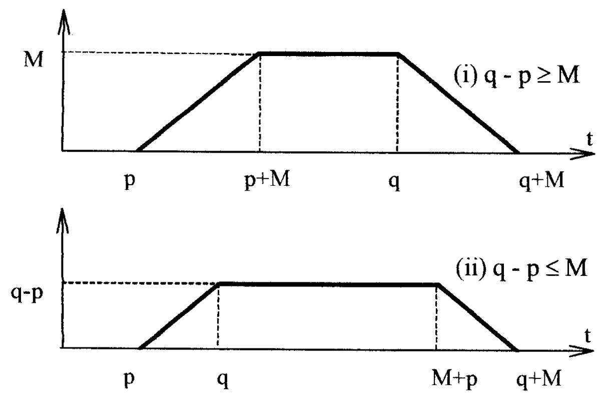

Figure 1. *Function* $w_{M,p,q}(t)$

We shall also need six matrices $B_1, \dots, B_6$ that are defined as follows.
Matrix B_1 is the diagonal matrix of size $(M+Q-1) \times (M+Q-1)$; its elements are

$$b_{ij}^{(1)} = \begin{cases} w_{M,0,Q}(i), & \text{if } i = j \\ 0, & \text{otherwise.} \end{cases} \tag{11}$$

Matrix B_2 is presented in *Figure 2*. It is an $(M+Q-1) \times (M+Q-1)$-matrix with $A = \min\{M, Q\}$. The elements of B_2 are

$$b_{ij}^{(2)} = \begin{cases} w_{i,0,A}(j), & 1 \le i < A \\ w_{A,0,A}(j), & A \le i < \max\{M, Q\} \\ w_{M+Q-i,i-A,i}(j), & \max\{M, Q\} \le i \le M+Q-1. \end{cases} \tag{12}$$

Matrix B_3 is the matrix V of *Figure 2*; its size is $(M+K-1) \times (M+K-1)$ and the parameters are $A = M$, $v_1 = v_2 = K$ and $a = M-1$. The elements of B_3 are

$$b_{ij}^{(3)} = \begin{cases} w_{i,0,K}(j), & \text{if } 1 \le i < M \\ w_{M,0,K}(j), & \text{if } M \le i < K \\ w_{M+K-i,i-K,i}(j), & \text{if } K \le i \le M + K - 1. \end{cases} \tag{13}$$

Matrix B_4 is the matrix U of *Figure 2* with $A = B = M$ and $u_1 = u_2 = K-M+1$. Its size is $(M+K-1) \times (M+K-1)$ and its elements are

$$b_{ij}^{(4)} = w_{M,0,K}(i) \times w_{M,0,K}(j), \tag{14}$$

where $1 \le i, j \le K+M-1$.

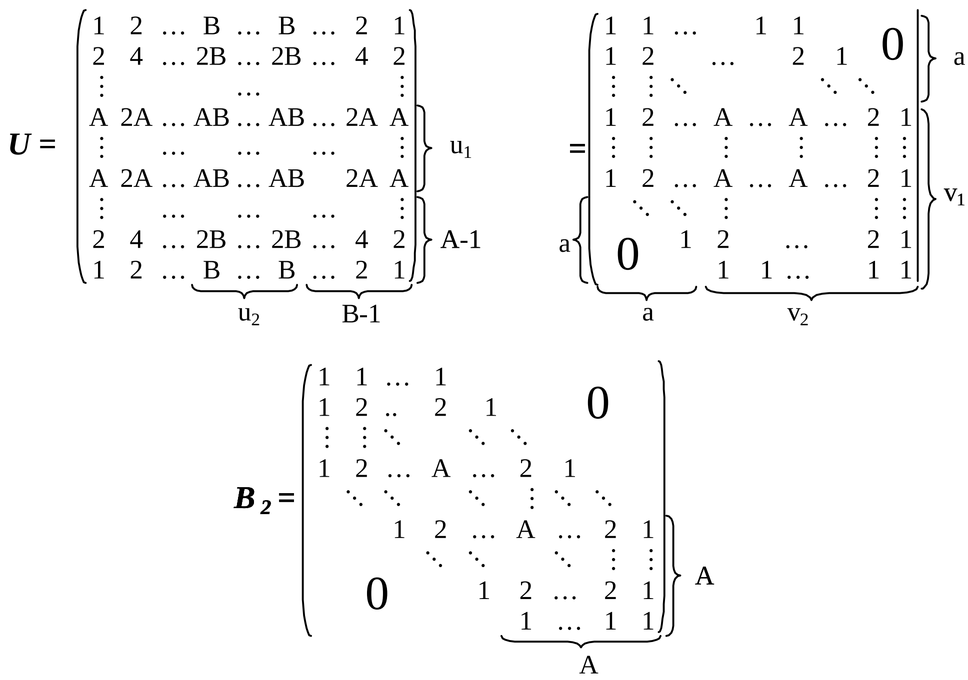

Figure 2. *Matrices U, V and B_2.*

Matrix B_5 is an $(M+K-1) \times (M+Q-1)$-matrix V (see *Figure 2*) with $A = \min\{M, Q\}$, $v_1 = K$, $v_1 = Q$, and $a = M-1$. The elements are

$$B_5 = b_{ij}^{(5)} = \begin{cases} w_{i,0,Q}(j), & \text{if } 1 \le i \le M \\ w_{M,0,Q}(j), & \text{if } M \le i \le K \\ w_{M+K-i,i-K,Q+i-K}(j), & \text{if } K \le i \le M+K-1. \end{cases}$$

Matrix B_6 is the matrix U with $A = M$, $B = \min\{M, Q\}$, $u_1 = K-M+1$ and $u_2 = | Q-M | +1$. Its size is $(M+K-1) \times (M+Q-1)$ and the elements are $b_{ij}^{(6)} = w_{M,0,K}(i) \times w_{M,0,Q}(j)$ for $1 \le i \le K+M-1$, $1 \le j \le Q+M-1$.

Finally, as an addition to (8), we define

$$\tilde{\varepsilon}_{i.} = \frac{1}{Q} \sum_{j=p+1}^{q} \varepsilon_{ij}, \quad \tilde{\varepsilon}_{..} = \frac{1}{MQ} \sum_{i=1}^{M} \sum_{j=p+1}^{q} \varepsilon_{ij} \tag{15}$$

2.2. The quadratic form

Theorem 1. *Let $y_t = a + bt + e_t$ for all $t = 1, 2, \dots$ and some a and b. Then the sum of squares $SS_{p,q}$ can be represented as a quadratic form*

$$SS_{p,q} = e^T B e \,,$$

where $e = (e_1, \ldots, e_{q+M-1})^T$ *and*

$$B = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & B_1 \end{pmatrix} - \frac{1}{M}\begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & B_2 \end{pmatrix} + \frac{Q}{K^2}\begin{pmatrix} B_3 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} - \frac{Q}{K^2M}\begin{pmatrix} B_4 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$$
$$-\frac{1}{K}\left[\begin{pmatrix} \mathbf{0} & B_5 \\ \mathbf{0} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ B_5^T & \mathbf{0} \end{pmatrix}\right] + \frac{1}{KM}\left[\begin{pmatrix} \mathbf{0} & B_6 \\ \mathbf{0} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ B_6^T & \mathbf{0} \end{pmatrix}\right]$$

The structure of the matrix B is represented in *Figure 3*, where zero is coded by white and different patterns in right bottom, left top, and left bottom corners correspond to the matrices $B_1 - \frac{1}{M}B_2$, $\frac{Q}{K^2}B_3 - \frac{Q}{K^2M}B_4$ and $-\frac{1}{K}B_5 + \frac{1}{KM}B_6$, respectively.

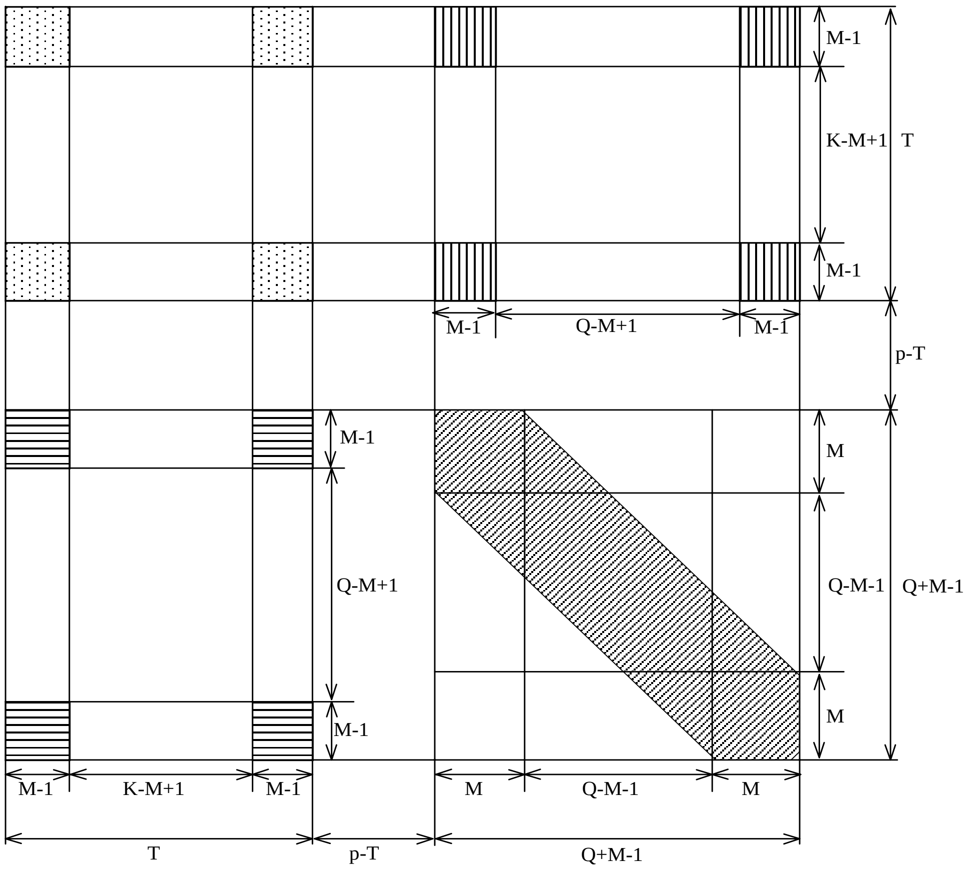

Figure 3. *Matrix B*

Proof of Theorem 1. According to the notations of (8) and (15) and the definition of the sum of squares (4), we have

$$SS_{p,q} = \sum_{i=1}^{M} \sum_{j=p+1}^{q} \left(\varepsilon_{ij} - \varepsilon_{.j} - \varepsilon_{i.} + \varepsilon_{..}\right)^2 .$$

Expanding the square and simplifying separately each term in the sum, we obtain

$$SS_{p,q} = S_1 - MS_2 + QS_3 - MQS_4 - 2QS_5 + 2MQS_6 \,, \tag{16}$$

where

$$S_1 = \sum_{i=1}^{M} \sum_{j=p+1}^{q} \varepsilon_{ij}^2 \,, \quad S_2 = \sum_{j=p+1}^{q} \varepsilon_{.j}^2 \,, \quad S_3 = \sum_{i=1}^{M} \varepsilon_{i.}^2 \,,$$

$$S_4 = \varepsilon_{..}^2 \,, \quad S_5 = \sum_{i=1}^{M} \tilde{\varepsilon}_{i.} \varepsilon_{i.} \,, \quad S_6 = \tilde{\varepsilon}_{..} \varepsilon_{..}$$

To see how the simplification is made, consider the three most difficult terms:

$$\sum_{i=1}^{M} \sum_{j=p+1}^{q} \varepsilon_{i.} \varepsilon_{.j} = \sum_{i=1}^{M} \varepsilon_{i.} \sum_{j=p+1}^{q} \varepsilon_{.j} = \left[\sum_{i=1}^{M} \frac{1}{K} \sum_{j=1}^{K} \varepsilon_{ij} \right] \left[\sum_{j=p+1}^{q} \frac{1}{M} \sum_{i=1}^{M} \varepsilon_{ij} \right] = M \varepsilon_{..} Q \tilde{\varepsilon}_{..} \,,$$

$$\sum_{i=1}^{M} \sum_{j=p+1}^{q} \varepsilon_{ij} \varepsilon_{.j} = M \sum_{j=p+1}^{q} \varepsilon_{.j} \left[\frac{1}{M} \sum_{i=1}^{M} \varepsilon_{ij} \right] = M \sum_{j=p+1}^{q} \varepsilon_{.j}^2 \,,$$

$$\sum_{i=1}^{M} \sum_{j=p+1}^{q} \varepsilon_{ij} \varepsilon_{i.} = Q \sum_{i=1}^{M} \varepsilon_{i.} \left[\frac{1}{Q} \sum_{j=p+1}^{q} \varepsilon_{ij} \right] = Q \sum_{i=1}^{M} \varepsilon_{i.} \tilde{\varepsilon}_{i.} \,.$$

Consider separately each sum in (16).

It is easy to see from (11) and (16) that

$$S_1 = e^T \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & B_1 \end{pmatrix} e \,.$$

Consider S_2 and replace $\varepsilon_{.j}$ by the corresponding expression from (8). Using the notation $\varepsilon_{ij} = e_{i+j-1}$ and $e = (e_{p+1} \ldots, e_{q+M-1})^T$ we have

$$S_2 = \sum_{j=p+1}^{q} \left(\frac{1}{M} \sum_{i=1}^{M} \varepsilon_{ij}\right)^2 = \frac{1}{M^2} \sum_{j=p+1}^{q} \sum_{i=1}^{M} \sum_{i'=1}^{M} e_{i+j-1} e_{i'+j-1} \,.$$

We now change the indices by the formula

$$\begin{cases} t = i + j - 1 \\ t' = i' + j - 1 \end{cases}$$

Since $i, i' = 1, \ldots, M$, $j = p+1, \ldots, q$ we have $t, t' = p+1, \ldots, q+M-1$. Therefore,

$$S_2 = \frac{1}{M^2} \left[\underbrace{\sum_{t=p+1}^{p+M} \sum_{t'=p+1}^{p+M} e_t e_{t'} + \sum_{t=p+2}^{p+M+1} \sum_{t'=p+2}^{p+M+1} e_t e_{t'} + \ldots + \sum_{t=q}^{q+M-1} \sum_{t'=q}^{q+M-1} e_t e_{t'}}_{q-p} \right]$$

$$= \frac{1}{M^2} e \left[\begin{pmatrix} \mathbf{1}_M & \mathbf{0}_{M,Q-1} \\ \mathbf{0}_{Q-1,M} & \mathbf{0}_{Q-1,Q-1} \end{pmatrix} + \begin{pmatrix} \mathbf{0}_{1,1} & \mathbf{0}_{1,M} & \mathbf{0}_{1,Q-2} \\ \mathbf{0}_{M,1} & \mathbf{1}_M & \mathbf{0}_{M,Q-2} \\ \mathbf{0}_{Q-2,1} & \mathbf{0}_{Q-2,M} & \mathbf{0}_{Q-2,Q-2} \end{pmatrix} \right.$$

$$\left. + \ldots + \begin{pmatrix} \mathbf{0}_{Q-2,Q-2} & \mathbf{0}_{Q-2,M} & \mathbf{0}_{Q-2,1} \\ \mathbf{0}_{M,Q-2} & \mathbf{1}_M & \mathbf{0}_{M,1} \\ \mathbf{0}_{1,Q-2} & \mathbf{0}_{1,M} & \mathbf{0}_{1,1} \end{pmatrix} + \begin{pmatrix} \mathbf{0}_{Q-1,Q-1} & \mathbf{0}_{Q-1,M} \\ \mathbf{0}_{M,Q-1} & \mathbf{1}_M \end{pmatrix} \right] e^T$$

where $\mathbf{1}_M$ is the $M \times M$-matrix of ones and $\mathbf{0}_{u,v}$ is the $u \times v$-matrix of zeros. Summing the matrices above we obtain the matrix B_2, see (12), and

$$MS_2 = \frac{1}{M} e^T \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & B_2 \end{pmatrix} e$$

Matrix B_3, see (13), is built from the sum of squares S_3 analogously to the construction of B_2 from S_2. In this case we use the substitution

$$\begin{cases} t = i + k - 1 \\ t' = i + k' - 1 \end{cases}$$

where $i = 1, \ldots, M,\ \ k, k' = 1, \ldots, K$ and $t, t' = 1, \ldots, K+M-1$. This gives

$$QS_3 = \frac{Q}{K^2} e^T \begin{pmatrix} B_3 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} e\,.$$

The sum of squares S_4 gives us the matrix $\frac{1}{K^2M^2} B_4$; this can be easily seen if we consider B_4 as a square of the $(M+K-1) \times (M+K-1)$-matrix with elements $w_{M,0,K}(i)$, if $i = j$, and 0, otherwise. Thus,

$$MQS_4 = \frac{Q}{K^2 M} e^T \begin{pmatrix} B_4 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} e$$

We can obtain the matrix B_5 similarly to the case of B_3 using the similarity between the sums of squares S_3 and S_5. In view of the differences in the number of terms in the sums $\tilde{\varepsilon}_{i.}$ and $\varepsilon_{i.}$, see (8) and (15), we obtain different sizes and multipliers. We thus have

$$2QS_5 = \frac{1}{K} e^T \left[\begin{pmatrix} \mathbf{0} & B_5 \\ \mathbf{0} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ B_5^T & \mathbf{0} \end{pmatrix} \right] e\,.$$

Finally, B_6 is an $(M+K-1) \times (M+Q-1)$-matrix which can be obtained similarly to B_4.

$$2MQS_6 = \frac{1}{KM} e^T \left[\begin{pmatrix} \mathbf{0} & B_6 \\ \mathbf{0} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ B_6^T & \mathbf{0} \end{pmatrix} \right] e\,.$$

This completes the proof. □

2.3. Computation of tr$\boldsymbol{B}$ and tr$\boldsymbol{B}^2$

As a corollary of *Theorem 1*, we can derive the expressions for tr$B$ and trB^2 in several particular cases, depending on the values of parameters p and q.

Case 1: $p \geq N$. We have

$$\mathrm{tr}B = \frac{Q(M-1)(3K^2+M+1)}{3K^2}$$

$$\mathrm{tr}B^2 = \frac{(2K^2+Q^2)(M^2-1)(2M^2+7)}{45K^4} + \frac{Q(M-1)(M^2-M-1)}{3M} - \frac{(M-1)(2M^2-M-3)}{6}.$$

Case 2: $p = 0$, $q = K$. In this case

$$SS_{p,q} = \sum_{i=1}^{M}\sum_{k=1}^{K}(\varepsilon_{ik} - \varepsilon_{.k} - \varepsilon_{i.} + \varepsilon_{..})^2 =$$

$$= \sum_{i=1}^{M}\sum_{k=1}^{K}\varepsilon_{ik}^2 - K\sum_{i=1}^{M}\varepsilon_{i.}^2 - M\sum_{k=1}^{K}\varepsilon_{.k}^2 + MK\varepsilon_{..}^2 = e^T Be$$

implying $Q = K$, $B_3 = B_5 = B_5^T$ and $B_4 = B_6 = B_6^T$; therefore, the matrix B has the form

$$B = B_1 - \frac{1}{M}B_2 + \frac{1}{K}B_3 - \frac{1}{MK}B_4\,.$$

For $i \leq j$ and $i + j \leq K + M$ we have

$$b_{ij} = \begin{cases} \frac{i(i+MK-M-K)}{MK}, & \text{if } i = j, 1 \leq i \leq M-1 \\ M-1, & \text{if } i = j, M \leq i \leq \frac{M+K}{2} \\ \frac{j-i}{M} - 1, & \text{if } M \leq j,\ \ j - M + 1 \leq i \leq j \\ -\frac{i(M+K-j)}{MK}, & \text{if } 1 \leq i < j \leq M-1 \\ \frac{i(M+K-j)}{MK}, & \text{if } K+1 \neq K+M-1,\ \ 1 \leq i \leq j-K \\ -\frac{(M-i)(j-K)}{MK}, & \text{if } K+1 \leq j \neq K+i,\ \ 1 \leq i \leq M-1 \\ 0, & \text{otherwise} \end{cases}$$

and $b_{ij} = b_{ji},\ b_{M+K-i,\,M+K-j} = b_{ij}$ for $1 \leq i \leq M+K-1,\ \ 1 \leq j \leq M+K-1$. This yields

$$\mathrm{tr}B = \frac{(M-1)(3K^2-M-1)}{3K}\,,$$

$$\mathrm{tr}B^2 = \frac{(M^2-1)(2M^2+7)}{45K^2} + \frac{K(M-1)(3M^2-M-1)}{3M} - \frac{(M^2-1)(2M-3)}{6} + \frac{(M^2-1)(2-3M^2)}{15KM}.$$

3. Single centring

Consider the case of single centring. Using the notation $\varepsilon_{ij} = e_{i+j-1}$ and (8) and (15) we obtain

$$SS_{p,q} = \sum_{i=1}^{M}\sum_{j=p+1}^{q}(\varepsilon_{ij} - \varepsilon_{i.})^2 = \sum_{i=1}^{M}\sum_{j=p+1}^{q}\varepsilon_{ij}^2 + Q\sum_{i=1}^{M}\varepsilon_{i.}^2 - 2Q\sum_{i=1}^{M}\tilde{\varepsilon}_{i.}\varepsilon_{i.}$$

This yields that the sum of squares $SS_{p,q}$ can again be represented as a quadratic form $e^T Be$, where the matrix B has the form

$$B = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & B_1 \end{pmatrix} + \frac{Q}{K^2}\begin{pmatrix} B_3 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} - \frac{1}{K}\left[\begin{pmatrix} \mathbf{0} & B_5 \\ \mathbf{0} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ B_5^T & \mathbf{0} \end{pmatrix}\right].$$

Here the matrices B_1, B_3, B_5 are described as above and $\mathbf{0}$ is the zero-matrix of suitable size.

Let us compute tr$B$ and trB^2 in the two particular cases as in *Section 2*.

Case 1: $p \geq N$. We have

$$\mathrm{tr}B = \frac{MQ(K+1)}{K};$$

$$\begin{aligned}\mathrm{tr}B^2 \quad = \quad & M^2Q - \frac{M(M^2-1)}{3} \\ & + \frac{Q^2}{K^4}[(K-M+1)^2M^2 - \frac{M(M-1)}{6}(5M^2 - 8KM - 7M + 4K)] \\ & + \frac{2}{K^2}[(K-M+1)(Q-M+1)M^2 \\ & - \frac{M(M-1)}{6}(5M^2 - 4M(K+Q) - 7M + 2(K+Q))]\end{aligned}$$

Case 2: $p = 0$, $q = K$. We have

$$e^TBe = SS_{p,q} = \sum_{i=1}^{M}\sum_{j=1}^{K}(\varepsilon_{ij} - \varepsilon_{i.})^2 = \sum_{i=1}^{M}\sum_{j=1}^{K}\varepsilon_{ij}^2 - K\sum_{i=1}^{M}\varepsilon_{i.}^2\,,$$

implying $Q = K$, $B_3 = B_5 = B_5^T$. Therefore, the matrix B has the form

$$B = B_1 - \frac{1}{K}B_3;$$

its elements are

$$b_{ij} = \begin{cases} \frac{K-1}{K}w_{M,O,K}(j), & \text{if } \ i = j \\ -\frac{1}{K}w_{i,\,0,\,K}(j), & \text{if } \ i \neq j, \ \ 1 \leq i \leq M \\ -\frac{1}{K}w_{M,\,0,\,K}(j), & \text{if } \ i \neq j, \ \ M \leq i \leq K \\ -\frac{1}{K}w_{M+K-i,\,i-K,\,i}(j), & \text{if } \ i \neq j \ \ K \leq i \leq M+K-1. \end{cases}$$

The expressions for tr$B$ and trB^2 are

$$\mathrm{tr}B = M(K-1), \ \ \mathrm{tr}B^2 = M^2K - \frac{M(M^2-1)}{3} - M^2 + \frac{M^2(M^2-1)}{6K^2}\,.$$

4. No centring

The case without averaging is the easiest. In this case we have

$$SS_{p,q} = \sum_{i=1}^{M}\sum_{j=p+1}^{q}\varepsilon_{ij}^2 = e^TBe, \quad \text{where} \quad B = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & B_1 \end{pmatrix},$$

$$\mathrm{tr}B = \sum_t w_{M,p,q}(t) = \sum_t w_{M,0,Q}(t) = MQ$$

and

$$\mathrm{tr}B^2 = \sum_t w^2_{M,p,q}(t) = \begin{cases} \frac{1}{3}M\left(3MQ + 1 - M^2\right), & \text{if } Q \geq M \\ \frac{1}{3}Q\left(3MQ + 1 - Q^2\right), & \text{if } Q \leq M\,. \end{cases}$$

In particular, for $p = 0$ and $q = K$ we have $B = B_1$,

$$\mathrm{tr}B = MK \quad \text{and} \quad \mathrm{tr}B^2 = M^2K - \frac{M(M^2-1)}{3}\,.$$

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