The Commutation Matrix: Some Properties and Applications

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THE COMMUTATION MATRIX: SOME PROPERTIES AND APPLICATIONS

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The commutation matrix K is defined as a square matrix containing only zeroes and ones. Its main properties are that it transforms vec$A$ into vecA', and that it reverses the order of a Kronecker product. An analytic expression for K is given and many further properties are derived. Subsequently, these properties are applied to some problems connected with the normal distribution. The expectation is derived of $\varepsilon'A\varepsilon \cdot \varepsilon'B\varepsilon \cdot \varepsilon'C\varepsilon$, where $\varepsilon \sim N(0, V)$, and A, B, C are symmetric. Further, the expectation and covariance matrix of $x \otimes y$ are found, where x and y are normally distributed dependent variables. Finally, the variance matrix of the (noncentral) Wishart distribution is derived.

1. Introduction. Tracy and Dwyer (1969) introduced a matrix that was later given the name "permuted identity matrix" by MacRae (1974). Its central property is that it transforms vec$A$ into vecA', where A is an arbitrary (m, n) matrix. We shall denote this matrix as K_{mn}. MacRae showed that K_{mn} can be used for reversing the order of a Kronecker product, a property very useful in the calculation of matrix derivatives. Barnett (1973) and Conlisk (1976) independently rediscovered this matrix. Balestra (1976), extending MacRae's paper, gives a great number of important results on K_{mn} in matrix differentiation.

In this paper we shall derive further properties of the commutation matrix, as we prefer to call it, and use these in some problems in statistics. We shall find expressions for the expectations and covariance matrices of stochastic vectors $x \otimes y$, where $x \sim N_n(\mu_1, V_1)$ and $y \sim N_m(\mu_2, V_2)$ are stochastically dependent, and $x \otimes x$, where $x \sim N_n(\mu, V)$. These results will then be applied to the central and noncentral Wishart distributions for which the variance matrices will be derived. Various related results will also be reported.

2. Definitions, basic results. Let $A = (a_{ij})$ be an (m, n) matrix and $A_{.j}$ the jth column of A; then vec$A$ is the (mn) column vector

$$\text{vec } A = \begin{bmatrix} A_{.1} \\ \vdots \\ A_{.n} \end{bmatrix}.$$

Let further B be an (s, t) matrix; then the Kronecker product $A \otimes B$ is defined as the (ms, nt) matrix

$$A \otimes B = (a_{ij}B).$$

The reader is assumed to be familiar with the basic properties of Kronecker products (see Neudecker (1968)). For easy reference we only state the following relations:

(2.1)
$$\text{vec } ABC = (C' \otimes A)\text{vec } B.$$

Let x and y be vectors of any order, then

(2.2)
$$x \otimes y = \text{vec } yx'$$

and

(2.3)
$$x \otimes y' = xy' = y' \otimes x.$$

The basic connection between the vec-function and the trace is

(2.4)
$$(\text{vec } A')'\text{vec } B = \text{tr } AB.$$

We shall also define the (m, n) matrix

(2.5)
$$H_{ij} = a_i e_j',$$

where a_i is the ith column unit vector of order m and e_j is the jth column unit vector of order n.

Clearly, any (m, n) matrix A can be written as

(2.6)
$$A = \Sigma_{ij} a_{ij} H_{ij}.$$

Finally we define the (n, n) matrix

(2.7)
$$E_{ij} = e_i e_j'.$$

From this definition it follows that

(2.8)
$$\Sigma_i E_{ii} = I_n.$$

Also, from (2.2), (2.7) and (2.8) we have

(2.9)
$$\text{vec } I_n = \Sigma_i (e_i \otimes e_i),$$

since

$$\text{vec } I_n = \text{vec } \Sigma_i E_{ii} = \text{vec } \Sigma_i e_i e_i' = \Sigma_i \text{vec } (e_i e_i') = \Sigma_i (e_i \otimes e_i).$$

Further,

(2.10)
$$E_{ij} \otimes E_{kl} = (\text{vec } E_{ki})(\text{vec } E_{lj})',$$

since

$$(\text{vec } E_{ki})(\text{vec } E_{lj})' = (\text{vec } e_k e_i')(\text{vec } e_l e_j')'$$
$$= (e_i \otimes e_k)(e_j \otimes e_l)' = (e_i e_j') \otimes (e_k e_l') = E_{ij} \otimes E_{kl}.$$

From (2.8) and (2.10) follows

(2.11)
$$\Sigma_{ij}(E_{ij} \otimes E_{ij}) = (\text{vec } I_n)(\text{vec } I_n)'.$$

3. Some properties of the commutation matrix. Let us now introduce the commutation matrix K_{mn} as the (mn, mn) matrix which, for arbitrary (m, n) matrix A, transforms vec$A$ into vecA'. It is easy to see that K_{mn} is unique. Its explicit form

can be derived as follows. Using (2.1), (2.5) and (2.6), we see that

$$\text{vec } A' = \text{vec } \Sigma_{ij} a_{ij} H'_{ij} = \text{vec } \Sigma_{ij}(a'_i A e_j)(e_j a'_i)$$

$$= \text{vec } \Sigma_{ij}(e_j a'_i A e_j a'_i)$$

$$= \Sigma_{ij}\text{vec } (H'_{ij} A H'_{ij}) = \Sigma_{ij}(H_{ij} \otimes H'_{ij})\text{vec } A.$$

Hence the following definition is put forward:

DEFINITION 3.1. The (mn, mn) commutation matrix K_{mn} is

$$K_{mn} = \Sigma_{i=1}^m \Sigma_{j=1}^n (H_{ij} \otimes H'_{ij}),$$

where H_{ij} is an (m, n) matrix with a 1 in its ijth position and zeroes elsewhere, i.e., $H_{ij} = a_i e'_j$, as defined in (2.5). For example,

$$K_{23} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

For notational brevity we shall write the (n^2, n^2) matrix K_{nn} as K_n.

In words, K_{mn} is a square mn-dimensional matrix partitioned into mn sub-matrices of order (n, m) such that the ijth submatrix has a 1 in its jith position and zeroes elsewhere. MacRae (1974, page 338) uses the symbol $I_{(n, m)}$ and Balestra (1976) uses $P_{n, m}$.

THEOREM 3.1.
   (i)
$$K_{mn} = \Sigma_{j=1}^n (e'_j \otimes I_m \otimes e_j) = \Sigma_{i=1}^m (a_i \otimes I_n \otimes a'_i),$$
where e_j and a_i are the unit vectors defined above;
   (ii) $K'_{mn} = K_{nm}$;
   (iii) $K'_{mn} K_{mn} = K_{mn} K'_{mn} = I_{mn}$, or $K_{mn}^{-1} = K_{nm}$;
   (iv) $K_{1n} = K_{n1} = I_n$;
   (v) tr $K_{mn} = 1 + d(m - 1, n - 1)$, where $d(m, n)$ is the greatest common divisor of m and n $(d(0, n) = d(n, 0) = n)$.
   (vi) The eigenvalues of K_n are $+1$ and -1 with multiplicities $\frac{1}{2}n(n + 1)$ and $\frac{1}{2}n(n - 1)$. $|K_n| = (-1)^{\frac{1}{2}n(n-1)}$. In general, $K_{mn}(m \neq n)$ will have some complex eigenvalues. $|K_{mn}| = (-1)^{\frac{1}{4}m(m-1)n(n-1)}$.
   (vii) $K_{mn}\text{vec } A = \text{vec } A'$, where A is an (m, n) matrix.
   (viii) $K_{mn}(A \otimes B)K_{st} = B \otimes A$, where A is an (n, s) matrix and B is an (m, t) matrix. Equivalently, $K_{mn}(A \otimes B) = (B \otimes A)K_{ts}$.
   (ix) Special cases of (viii) are $K_{mn}(A \otimes B) = (B \otimes A)K_{mn}$, where A and B are

square matrices of order n and m respectively. Also

$$K_{mn}(Y \otimes x) = x \otimes Y,$$

$$(Y \otimes x')K_{sm} = x' \otimes Y,$$

$$K_{mn}(y \otimes x) = x \otimes y,$$

where Y is an (n, s) matrix, y is an n-vector, and x is an m-vector.

    (x) *Let P and Q be matrices with m and n rows respectively, x is an m-vector, y is an n-vector, and z is arbitrary. Then,*

$$z' \otimes P \otimes y = K_{mn}(yz' \otimes P)$$

$$x \otimes Q \otimes z' = K_{mn}(Q \otimes xz').$$

    (xi) *The matrix $K_{st,\,n}$ (which denotes K_{mn} with $m = st$) was introduced by Balestra (1976). It performs a cyclic permutation of the Kronecker product of three matrices:*

$$A \otimes B \otimes C = K_{ms,\,p}(C \otimes A \otimes B)K_{q,\,tn} = K_{m,\,sp}(B \otimes C \otimes A)K_{qt,\,n},$$

where A, B and C are matrices of orders (m, n), (s, t), and (p, q) respectively. Also,

$$K_{ts,\,n}K_{sn,\,t}K_{nt,\,s} = I_{tsn}.$$

Any two K-matrices with the same set of three indices commute (e.g., $K_{st,\,n}K_{t,\,sn} = K_{t,\,sn}K_{st,\,n}$).

    (xii) *Define the (m, n) matrix A, the (p, q) matrix B, the (q, s) matrix C, and the (n, t) matrix D. Then,*

$$K_{mp}(BC \otimes AD) = (A \otimes B)K_{nq}(C \otimes D) = (AD \otimes BC)K_{ts}$$

$$= (I_m \otimes BC)K_{ms}(I_s \otimes AD) = (AD \otimes I_p)K_{tp}(BC \otimes I_t).$$

    (xiii) $\operatorname{tr} K_{mn}(A' \otimes B) = \operatorname{tr} A'B = (\operatorname{vec} A')'K_{mn}(\operatorname{vec} B)$, *where A and B are (m, n) matrices.*

    (xiv) *Let A be an (m, n) matrix with rank r. Denote the r nonzero (hence positive) eigenvalues of $A'A$ as $\lambda_1 \cdots \lambda_r$, and define*

$$P = K_{mn}(A' \otimes A).$$

    Then, P is a symmetric matrix with rank r^2, $\operatorname{tr} P = \operatorname{tr}(A'A)$. Further, $P^2 = (AA') \otimes (A'A)$. The nonzero eigenvalues of P are $\lambda_1 \cdots \lambda_r$ and $\pm(\lambda_i\lambda_j)^{\frac{1}{2}}$ $(i \neq j)$.

PROOF.

    (i) $K_{mn} = \Sigma_{ij}(H_{ij} \otimes H'_{ij}) = \Sigma_{ij}(a_i e'_j \otimes e_j a'_i).$

Using (2.3) we see that

$$\Sigma_{ij}(a_i e'_j \otimes e_j a'_i) = \Sigma_{ij}(e'_j \otimes a_i \otimes a'_i \otimes e_j) = \Sigma_j(e'_j \otimes (\Sigma_i a_i \otimes a'_i) \otimes e_j)$$

$$= \Sigma_j(e'_j \otimes (\Sigma_i a_i a'_i) \otimes e_j) = \Sigma_j(e'_j \otimes I_m \otimes e_j).$$

Also,

$$\Sigma_{ij}(a_i e'_j \otimes e_j a'_i) = \Sigma_{ij}(a_i \otimes e'_j \otimes e_j \otimes a'_i) = \Sigma_i(a_i \otimes (\Sigma_j e'_j \otimes e_j) \otimes a'_i)$$

$$= \Sigma_i(a_i \otimes (\Sigma_j e_j e'_j) \otimes a'_i) = \Sigma_i(a_i \otimes I_n \otimes a'_i).$$

(ii) $$K'_{mn} = \Sigma_{ij}(a_i e'_j \otimes e_j a'_i)' = \Sigma_{ji}(e_j a'_i \otimes a_i e'_j) = K_{nm}.$$

(iii) $$K'_{mn} K_{mn} = \Sigma_{ji}(e_j a'_i \otimes a_i e'_j)\Sigma_{st}(a_s e'_t \otimes e_t a'_s) = \Sigma_{jist}(e_j a'_i a_s e'_t \otimes a_i e'_j e_t a'_s)$$

$$= \Sigma_{ji}(e_j e'_j \otimes a_i a'_i) = (\Sigma_j e_j e'_j) \otimes (\Sigma_i a_i a'_i) = I_{mn}.$$

Hence, $K_{nm} = K'_{mn} = K^{-1}_{mn}$ or $K_{mn} K'_{mn} = I_{mn}$.

(iv) $$K_{1n} = \Sigma_j(e'_j \otimes e_j) = I_n = \Sigma_j(e_j \otimes e'_j) = K_{n1}.$$

(v) Clearly, from (iv), tr $K_{1n} = n$ and tr $K_{m1} = m$. The case where $m, n \geqslant 2$ is less trivial:

$$\text{tr } K_{mn} = \text{tr } \Sigma_{ij}(a_i e'_j \otimes e_j a'_i) = \Sigma_{ij} \text{tr}(a_i \otimes e_j)(e'_j \otimes a'_i) = \Sigma_{ij}(e_j \otimes a_i)'(a_i \otimes e_j).$$

Now, $(e_j \otimes a_i)$ is an mn-vector with unity in its $[(j-1)m+i]$th position and zeroes elsewhere. Similarly, $(a_i \otimes e_j)$ is an mn-vector with unity in its $[(i-1)n+j]$th position and zeroes elsewhere. Hence,

$$(e_j \otimes a_i)'(a_i \otimes e_j) \begin{array}{l} = 1 \quad \text{if} \quad (j-1)m+i = (i-1)n+j \\ = 0 \quad \text{otherwise.} \end{array}$$

Let $B[x_i | i = 1, \cdots, p]$ denote the number of cases where $x_i, i = 1, \cdots, p$ is true, then

$$\text{tr } K_{mn} = \Sigma^m_{i=1} \Sigma^n_{j=1}(e_j \otimes a_i)'(a_i \otimes e_j)$$

$$= B[(j-1)m+i = (i-1)n+j | i = 1 \cdots m, j = 1 \cdots n]$$

$$= B[(j-1)(m-1) = (i-1)(n-1) | i = 1 \cdots m, j = 1 \cdots n]$$

$$= 1 + B[(j-1)(m-1) = (i-1)(n-1) | i = 2 \cdots m, j = 2 \cdots n]$$

$$= 1 + B[j(m-1) = i(n-1) | i = 1 \cdots m-1, j = 1 \cdots n-1]$$

$$= 1 + B[(m-1)/(n-1) = i/j | i = 1 \cdots m-1, j = 1 \cdots n-1]$$

$$= 1 + d(m-1, n-1).$$

The last step follows from the following argument: let $m' = m/d(m, n)$ and $n' = n/d(m, n)$. Any combination (i, j) that satisfies $i/j = m/n$ $(i = 1 \cdots m, j = 1 \cdots n)$ must be of the form $i = \alpha m'$ and $j = \alpha n'$, where α is some positive rational number smaller than or equal to $d(m, n)$. Write $\alpha = p/q$, where p and q are positive integers with greatest common divisor (gcd) 1. Then, $i = pm'/q$ and $j = pn'/q$. For i and j to be positive integers it is necessary (and sufficient) that pm' and pn' are both divisible by q. Now, p and q have gcd 1 and the only common divisor of m' and n' is unity. Therefore $q = 1$. This implies that $i = pm'$ and $j = pn'$, $1 \leqslant p \leqslant d(m, n)$. Thus there are $d(m, n)$ combinations (i, j) for which $i/j = m/n$ $(i = 1 \cdots m, j = 1 \cdots n)$, i.e., $B[m/n = i/j | i = 1 \cdots m, j = 1 \cdots n] = d(m, n)$.

(vi) Since K_n is real orthogonal and symmetric, it has eigenvalues $+1$ and -1 only. Suppose the multiplicity of -1 is p. Then the multiplicity of $+1$ is $(n^2 - p)$

and $|K_n| = (-1)^p$. Also, using (v),

$$n = \text{tr } K_n = \text{sum of eigenvalues of } K_n = -p + n^2 - p = n^2 - 2p,$$

which implies $p = \frac{1}{2}n(n-1)$. In order to find $|K_{mn}|$ we write K_{mn} as (this proof was suggested by Pietro Balestra in a private communication to one of the authors):

$$K_{mn} = \Sigma_{j=1}^n (e_j' \otimes I_m \otimes e_j)$$

Now perform the following column-permutations: for $h = 1, 2, \cdots, n-1$, put the $[(n-h)m]$th column in the $(nm-h)$th position (this involves $(m-1)h$ permutations). Then, after $(m-1)[1 + 2 + \cdots + (n-1)] = \frac{1}{2}n(n-1)(m-1)$ permutations we have the following matrix:

Clearly, this is

$$\begin{bmatrix} K_{m-1,\,n} & 0 \\ 0 & I_n \end{bmatrix}$$

and therefore

$$|K_{mn}| = (-1)^{\frac{1}{2}n(n-1)(m-1)}|K_{m-1,\,n}| = \cdots = (-1)^{\frac{1}{2}n(n-1)[(m-1)+(m-2)+\cdots+1]}|K_{1n}|$$

$$= (-1)^{\frac{1}{2}n(n-1)\cdot\frac{1}{2}m(m-1)}|I_n| = (-1)^{\frac{1}{4}n(n-1)m(m-1)}.$$

(vii) In the beginning of this section we have already seen that $K_{mn} \text{vec} A = \text{vec} A'$.

(viii) Let X be an arbitrary (s, t)-matrix. Then, by repeated application of (vii) and (2.1),

$$K_{mn}(A \otimes B)K_{st}\text{vec } X = K_{mn}(A \otimes B)\text{vec } X' = K_{mn}\text{vec } BX'A'$$

$$= \text{vec } AXB' = (B \otimes A)\text{vec } X.$$

This holds for every X. Hence the first result. Postmultiplication with K_{ts} gives the second result.

(ix) The special cases follow from (viii) by putting ($t = m$ and $s = n$); $t = 1$; $m = 1$; and $s = t = 1$ respectively.

(x) Using (i) we have

$$K'_{mn}(z' \otimes P \otimes y) = \Sigma_j(e'_j \otimes I_m \otimes e_j)'(z' \otimes P \otimes y) = \Sigma_j(e_jz') \otimes P \otimes (e'_jy)$$

$$= \Sigma_j(e_i(e'_jy)z') \otimes P = ((\Sigma_je_je'_j)yz') \otimes P = yz' \otimes P.$$

Similarly,

$$K'_{mn}(x \otimes Q \otimes z') = \Sigma_i(a_i \otimes I_n \otimes a'_i)'(x \otimes Q \otimes z') = \Sigma_i(a'_ix) \otimes Q \otimes (a_iz')$$

$$= \Sigma_i(Q \otimes a_i(a'_ix)z') = Q \otimes (\Sigma_ia_ia'_i)xz' = Q \otimes xz'.$$

Premultiplication with K_{mn} gives the desired results.

(xi) The first result follows from the fact that the order of the Kronecker products in $(A \otimes B) \otimes C$ and $A \otimes (B \otimes C)$ can be reversed using (viii). Further,

$$K_{ts,\,n} = \Sigma^n_{j=1}(e'_j \otimes I_{st} \otimes e_j) = \Sigma_j(e'_j \otimes I_s) \otimes (I_t \otimes e_j)$$

$$= \Sigma_jK_{s,\,nt}[(I_t \otimes e_j) \otimes (e'_j \otimes I_s)]K_{t,\,sn} \quad \text{(by (viii))}$$

$$= \Sigma_jK_{s,\,nt}[I_t \otimes (e_je'_j) \otimes I_s]K_{t,\,sn} = K_{s,\,nt}K_{t,\,sn}.$$

Hence, by (iii), $K_{ts,\,n}K_{sn,\,t}K_{nt,\,s} = I_{tsn}$. Also, since $K_{ts,\,n} = K_{st,\,n}$,

$$K_{s,\,nt}K_{t,\,sn} = K_{ts,\,n} = K_{st,\,n} = K_{t,\,sn}K_{s,\,nt},$$

from which it follows that $K_{s,\,nt}$ and $K_{t,\,sn}$ commute. Clearly, this holds for any permutation of the indices s, n, t.

(xii) The result follows from repeated application of (viii):

$$(A \otimes B)K_{nq}(C \otimes D) = K_{mp}(B \otimes A)(C \otimes D) = K_{mp}(BC \otimes AD)$$

$$= K_{mp}(BC \otimes I_m)(I_s \otimes AD) = (I_m \otimes BC)K_{ms}(I_s \otimes AD).$$

Also,

$$(AD \otimes BC)K_{ts} = K_{mp}(BC \otimes AD) = K_{mp}(I_p \otimes AD)(BC \otimes I_t)$$

$$= (AD \otimes I_p)K_{tp}(BC \otimes I_t).$$

(xiii)

$$\text{tr } K_{mn}(A' \otimes B) = \Sigma_{ij}\text{tr}(H_{ij} \otimes H'_{ij})(A' \otimes B) = \Sigma_{ij}(\text{tr } H_{ij}A')(\text{tr } H'_{ij}B)$$

$$= \Sigma_{ij}(e'_jA'a_i)(a'_iBe_j) = \Sigma_{ij}a_{ij}b_{ij} = \text{tr } A'B.$$

Also, by (vii) and (2.4):

$$(\text{vec } A')'K_{mn} \text{ vec } B = (\text{vec } A)'\text{vec } B = \text{tr } A'B.$$

(xiv) $P' = (A \otimes A')K_{nm} = K_{mn}(A' \otimes A) = P$, by (viii). Hence P is symmetric. Since K_{mn} is nonsingular we have

$$\text{rank}(P) = \text{rank}(A' \otimes A) = \text{rank}(A') \cdot \text{rank}(A) = r^2.$$

Further, tr $P = \text{tr}(A'A)$ by (xiii).

$$P^2 = P'P = (A \otimes A')K_{nm}K_{mn}(A' \otimes A) = (A \otimes A')(A' \otimes A) = (AA') \otimes (A'A).$$

Hence, the r^2 nonzero eigenvalues of P^2 are $\lambda_i \lambda_j$ ($i, j = 1 \cdots r$). Each nonzero eigenvalue of P must then be of the form $\pm (\lambda_i \lambda_j)^{\frac{1}{2}}$. The sum of these r^2 eigenvalues is $\text{tr} P = \text{tr}(A'A) = \sum_{i=1}^{r} \lambda_i$. The nonzero eigenvalues of P are thus λ_i ($i = 1 \cdots r$) and $\pm (\lambda_i \lambda_j)^{\frac{1}{2}}$ ($i \neq j = 1 \cdots r$).

4. Applications related to the normal distribution. In this section u will be a vector of n normally distributed independent stochastic variables u_i with $Eu_i = 0$ and $Eu_i^2 = 1$, i.e., $u \sim N(0, I_n)$. Further we define the symmetric matrices

$$(4.1) \qquad T_{ij} = E_{ij} + E_{ji}.$$

Hence $T_{ii} = 2E_{ii}$. We shall first prove the following

THEOREM 4.1.
(i) $E(uu' \otimes uu') = I \otimes I + \frac{1}{2} \Sigma_{ij} (T_{ij} \otimes T_{ij}) = I + K_n + (\text{vec } I)(\text{vec } I)'$;
(ii) $E(uu' \otimes uu' \otimes uu') = I \otimes I \otimes I + \frac{1}{2} \Sigma_{ij} [I \otimes T_{ij} \otimes T_{ij} + T_{ij} \otimes I \otimes T_{ij} + T_{ij} \otimes T_{ij} \otimes I] + \Sigma_{ijk} (T_{ij} \otimes T_{ik} \otimes T_{jk})$.

PROOF.   We know that

$$Eu_i = Eu_i^3 = Eu_i^5 = 0$$

and

$$Eu_i^2 = 1, \quad Eu_i^4 = 3, \quad Eu_i^6 = 15.$$

Clearly,

$$Eu_i u_j uu' = T_{ij} + \delta_{ij} I,$$

where δ_{ij} is the Kronecker delta:

$$\delta_{ij} \begin{array}{ll} = 1 & \text{if } i = j \\ = 0 & \text{if } i \neq j \end{array}.$$

Then

$$Euu' \otimes uu' = \Sigma_{ij} \big(E_{ij} \otimes (T_{ij} + \delta_{ij} I) \big) = \Sigma_{ij} (E_{ij} \otimes T_{ij}) + \Sigma_{ij} (\delta_{ij} E_{ij} \otimes I)$$

$$= \tfrac{1}{2} \Sigma_{ij} (T_{ij} \otimes T_{ij}) + (\Sigma_i E_{ii}) \otimes I = \tfrac{1}{2} \Sigma_{ij} (T_{ij} \otimes T_{ij}) + I \otimes I,$$

because $\Sigma_i E_{ii} = I$. Alternatively,

$$\Sigma_{ij} (E_{ij} \otimes T_{ij}) = \Sigma_{ij} (E_{ij} \otimes E_{ji}) + \Sigma_{ij} (E_{ij} \otimes E_{ij}) = K_n + (\text{vec } I)(\text{vec } I)',$$

according to (2.11).

In order to prove (ii) we need the following expectations:

$$
\begin{array}{ll}
Eu_i u_j u_h u_k uu' = 0, & i \neq j \neq h \neq k \\
\qquad\qquad = T_{hk}, & i = j, i \neq h \neq k \\
\qquad\qquad = I + T_{ii} + T_{hh}, & i = j, h = k, i \neq h \\
\qquad\qquad = 3 T_{ik}, & i = j = h, i \neq k \\
\qquad\qquad = 3I + 6 T_{ii}, & i = j = h = k.
\end{array}
$$

Thus,

$$Eu_i^2(uu' \otimes uu') = \tfrac{1}{2}\Sigma_{hk}(T_{hk} \otimes T_{hk}') + I \otimes T_{ii} + I \otimes I + T_{ii} \otimes I + 2\Sigma_k(T_{ik} \otimes T_{ik})$$

and

$$Eu_iu_j(uu' \otimes uu') = I \otimes T_{ij} + \Sigma_k(T_{ik} \otimes T_{jk}) + \Sigma_k(T_{jk} \otimes T_{ik}) + T_{ij} \otimes I \ (i \neq j).$$

This leads to

$$Eu_iu_juu' \otimes uu' = \delta_{ij}\Big[I \otimes I + \tfrac{1}{2}\Sigma_{hk}(T_{hk} \otimes T_{hk})\Big] + I \otimes T_{ij} + T_{ij} \otimes I$$
$$+ \Sigma_k(T_{ik} \otimes T_{jk}) + \Sigma_k(T_{jk} \otimes T_{ik}),$$

so that

$$E(uu' \otimes uu' \otimes uu') = \Sigma_{ij}\big(E_{ij} \otimes \big[Eu_iu_j(uu' \otimes uu')\big]\big)$$
$$= \Sigma_i\Big(E_{ii} \otimes \big[I \otimes I + \tfrac{1}{2}\Sigma_{hk}(T_{hk} \otimes T_{hk})\big]\Big)$$
$$+ \Sigma_{ij}(E_{ij} \otimes I \otimes T_{ij}) + \Sigma_{ij}(E_{ij} \otimes T_{ij} \otimes I)$$
$$+ \Sigma_{ijk}\big(E_{ij} \otimes \big[T_{ik} \otimes T_{jk} + T_{jk} \otimes T_{ik}\big]\big)$$
$$= I \otimes I \otimes I + \tfrac{1}{2}\Sigma_{ij}(I \otimes T_{ij} \otimes T_{ij}) + \tfrac{1}{2}\Sigma_{ij}(T_{ij} \otimes I \otimes T_{ij})$$
$$+ \tfrac{1}{2}\Sigma_{ij}(T_{ij} \otimes T_{ij} \otimes I) + \Sigma_{ijk}(T_{ij} \otimes T_{ik} \otimes T_{jk}).$$

This concludes the proof.

Theorem (4.1) enables us to give a simple proof of a result obtained by Neudecker (1968, pages 78–82). Also, his result is generalized. A still more general result is available in Magnus (1978), where, along different lines, a formula is derived for the expectation of an arbitrary number of quadratic forms in normally distributed variables.

THEOREM 4.2. *Let A, B and C be symmetric matrices of order n and* $\varepsilon \sim N_n(0, V)$, *where V is positive definite, then*

(i) $E(\varepsilon'A\varepsilon \cdot \varepsilon'B\varepsilon) = (\operatorname{tr} AV)(\operatorname{tr} BV) + 2 \operatorname{tr} AVBV.$

(ii) $E(\varepsilon'A\varepsilon \cdot \varepsilon'B\varepsilon \cdot \varepsilon'C\varepsilon) = (\operatorname{tr} AV)(\operatorname{tr} BV)(\operatorname{tr} CV) + 2[(\operatorname{tr} AV)(\operatorname{tr} BVCV) + (\operatorname{tr} BV)(\operatorname{tr} AVCV) + (\operatorname{tr} CV)(\operatorname{tr} AVBV)] + 8 \operatorname{tr} AVBVCV.$

PROOF. Let $u = V^{-\frac{1}{2}}\varepsilon$, then $u \sim N(0, I_n)$. Further, let $\bar{A} = V^{\frac{1}{2}}AV^{\frac{1}{2}}$, $\bar{B} = V^{\frac{1}{2}}BV^{\frac{1}{2}}$, and $\bar{C} = V^{\frac{1}{2}}CV^{\frac{1}{2}}$.

$$E(\varepsilon'A\varepsilon \cdot \varepsilon'B\varepsilon) = E\big(u'V^{\frac{1}{2}}AV^{\frac{1}{2}}u \cdot u'V^{\frac{1}{2}}BV^{\frac{1}{2}}u\big) = E(u'\bar{A}u \cdot u'\bar{B}u)$$
$$= E(u' \otimes u')(\bar{A} \otimes \bar{B})(u \otimes u) = \operatorname{tr}\big[(\bar{A} \otimes \bar{B})E(uu' \otimes uu')\big]$$
$$= \operatorname{tr}\big[(\bar{A} \otimes \bar{B})\big[I \otimes I + \tfrac{1}{2}\Sigma_{ij}(T_{ij} \otimes T_{ij})\big]\big]$$
$$= \operatorname{tr}(\bar{A} \otimes \bar{B}) + \tfrac{1}{2}\Sigma_{ij} \operatorname{tr}\big(\bar{A}T_{ij} \otimes \bar{B}T_{ij}\big)$$
$$= (\operatorname{tr} \bar{A})(\operatorname{tr} \bar{B}) + \tfrac{1}{2}\Sigma_{ij}\big(\operatorname{tr} \bar{A}T_{ij}\big)\big(\operatorname{tr} \bar{B}T_{ij}\big)$$
$$= (\operatorname{tr} \bar{A})(\operatorname{tr} \bar{B}) + \tfrac{1}{2}\Sigma_{ij}\big(2\bar{a}_{ij} \cdot 2\bar{b}_{ij}\big)$$
$$= (\operatorname{tr} \bar{A})(\operatorname{tr} \bar{B}) + 2\Sigma_{ij}\bar{a}_{ij}\bar{b}_{ij} = (\operatorname{tr} \bar{A})(\operatorname{tr} \bar{B}) + 2 \operatorname{tr} \bar{A}\bar{B}$$
$$= (\operatorname{tr} AV)(\operatorname{tr} BV) + 2 \operatorname{tr} AVBV.$$

Similarly,

$$E(\varepsilon'A\varepsilon \cdot \varepsilon'B\varepsilon \cdot \varepsilon'C\varepsilon) = E(u'\bar{A}u \cdot u'\bar{B}u \cdot u'\bar{C}u)$$
$$= \text{tr}\left[(\bar{A} \otimes \bar{B} \otimes \bar{C})E(uu' \otimes uu' \otimes uu')\right].$$

A straightforward application of result (ii) of Theorem 4.1 concludes the proof. Without proof we state the following corollary to Theorem 4.2.

COROLLARY 4.1.
(i) $\text{Cov}(\varepsilon'A\varepsilon, \varepsilon'B\varepsilon) = 2 \text{ tr } AVBV$,
(ii) $\text{Var}(\varepsilon'A\varepsilon) = 2 \text{ tr}(AV)^2$,
(iii) $E(\varepsilon'A\varepsilon)^3 = (\text{tr } AV)^3 + 6(\text{tr } AV)(\text{tr}(AV)^2) + 8 \text{ tr}(AV)^3$,
(iv) $\text{Cov}[(\varepsilon'A\varepsilon)^2, \varepsilon'B\varepsilon] = 4(\text{tr } AV)(\text{tr } AVBV) + 8 \text{ tr}(AV)^2BV$.

In many instances we need the variances and covariances of the elements of the stochastic matrix xx', or, somewhat more general, yx', where $x \sim N(\mu_1, V_1)$ and $y \sim N(\mu_2, V_2)$ may be correlated. An obvious example is the Wishart distribution. The following theorem gives these (co)variances and some related results.

THEOREM 4.3.   *Let the n-vector x and the m-vector y be jointly normally distributed. Let $z' = (x', y')$ and assume that*

$$Ez = \bar{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \quad and \, \text{Var}(z) = \bar{V} = \begin{pmatrix} P & Q' \\ Q & R \end{pmatrix},$$

where $\bar{V}$ is positive definite (hence nonsingular). Then,
(i) $E(x \otimes y) = \text{vec } Q + \mu_1 \otimes \mu_2$;
(ii) $\text{Var}(x \otimes y) = P \otimes R + P \otimes \mu_2\mu_2' + \mu_1\mu_1' \otimes R$
$\qquad\qquad\qquad + K_{nm}(Q \otimes Q' + Q \otimes \mu_1\mu_2' + \mu_2\mu_1' \otimes Q')$
$\qquad\qquad = (Exx') \otimes (Eyy') + K_{nm}((Eyx') \otimes (Exy')) - 2\mu_1\mu_1' \otimes \mu_2\mu_2'$;
(iii) $\text{tr}(\text{Var}(x \otimes y)) = (\text{tr}P)(\text{tr}R) + \text{tr}Q'Q + \mu_1'\mu_1(\text{tr}R) + \mu_2'\mu_2(\text{tr}P) + 2\mu_1'Q'\mu_2$.
Further, if x is distributed $N_n(\mu, V)$, V positive definite, then
(iv) $\text{Var}(x \otimes x) = (I + K_n)(V \otimes V + V \otimes \mu\mu' + \mu\mu' \otimes V)$;
(v) $\text{rank}(\text{Var}(x \otimes x)) = \frac{1}{2}n(n + 1)$.

Before giving the proof of the theorem, we shall prove the following simple lemma.

LEMMA 4.1.   *Let $u \sim N(0, I_n)$, then*
(i) $E(u \otimes u) = \text{vec } I_n$,
(ii) $\text{Var}(u \otimes u) = I + K_n$.

PROOF.

$$E(u \otimes u) = E \text{ vec } uu' = \text{vec } Euu' = \text{vec } I.$$

$$\text{Var}(u \otimes u) = E(uu' \otimes uu') - (\text{vec } I)(\text{vec } I)'$$
$$= I \otimes I + K_n + (\text{vec } I)(\text{vec } I)' - (\text{vec } I)(\text{vec } I)' = I + K_n,$$

according to Theorem 4.1. This proves (ii).

PROOF OF THEOREM 4.3.

$$E(x \otimes y) = E \operatorname{vec} yx' = \operatorname{vec} Eyx' = \operatorname{vec} \left[Q + (Ey)(Ex)' \right]$$

$$= \operatorname{vec} Q + \operatorname{vec} \mu_2 \mu_1' = \operatorname{vec} Q + \mu_1 \otimes \mu_2.$$

Define $w = \overline{V}^{-\frac{1}{2}}(z - \bar{\mu})$ and partition

$$\overline{V}^{\frac{1}{2}} = \begin{matrix} n \\ m \end{matrix} \left[\begin{matrix} Z_1 \\ Z_2 \end{matrix} \right].$$

Now,

$$w \sim N(0, I_{n+m})$$

and

$$\left[\begin{matrix} P & Q' \\ Q & R \end{matrix} \right] = \overline{V} = \overline{V}^{\frac{1}{2}} \overline{V}^{\frac{1}{2}} = \left[\begin{matrix} Z_1 Z_1' & Z_1 Z_2' \\ Z_2 Z_1' & Z_2 Z_2' \end{matrix} \right].$$

Further,

$$\binom{x}{y} = z = \overline{V}^{\frac{1}{2}} w + \bar{\mu} = \left[\begin{matrix} Z_1 \\ Z_2 \end{matrix} \right] w + \left[\begin{matrix} \mu_1 \\ \mu_2 \end{matrix} \right] = \left[\begin{matrix} Z_1 w + \mu_1 \\ Z_2 w + \mu_2 \end{matrix} \right].$$

Thus,

$$x \otimes y = (Z_1 w + \mu_1) \otimes (Z_2 w + \mu_2)$$

$$\operatorname{Var}(x \otimes y) = \operatorname{Var}\left[(Z_1 w \otimes Z_2 w) + (Z_1 w \otimes \mu_2) + (\mu_1 \otimes Z_2 w) + (\mu_1 \otimes \mu_2) \right]$$

$$= \operatorname{Var}\left[(Z_1 \otimes Z_2)(w \otimes w) + (Z_1 w \otimes \mu_2) + (\mu_1 \otimes Z_2 w) \right]$$

$$= \operatorname{Var}\left[(Z_1 \otimes Z_2)(w \otimes w) \right] + \operatorname{Var}(Z_1 w \otimes \mu_2) + \operatorname{Var}(\mu_1 \otimes Z_2 w)$$

$$+ E(Z_1 w \otimes \mu_2)(\mu_1 \otimes Z_2 w)' + E(\mu_1 \otimes Z_2 w)(Z_1 w \otimes \mu_2)'$$

$$= (Z_1 \otimes Z_2)\operatorname{Var}(w \otimes w)(Z_1 \otimes Z_2)' + E(Z_1 w \otimes \mu_2)(Z_1 w \otimes \mu_2)'$$

$$+ E(\mu_1 \otimes Z_2 w)(\mu_1 \otimes Z_2 w)' + E(\mu_1 \otimes Z_2 w)(Z_1 w \otimes \mu_2)'$$

$$+ \left[E(\mu_1 \otimes Z_2 w)(Z_1 w \otimes \mu_2)' \right]'$$

$$= (Z_1 \otimes Z_2)(I + K_{n+m})(Z_1 \otimes Z_2)' + Z_1 Z_1' \otimes \mu_2 \mu_2' + \mu_1 \mu_1' \otimes Z_2 Z_2'$$

$$+ E(\mu_1(Z_1 w)' \otimes Z_2 w \mu_2') + \left[E(\mu_1(Z_1 w)' \otimes Z_2 w \mu_2') \right]',$$

according to Lemma 4.1. Further,

$$(Z_1 \otimes Z_2)(I + K_{n+m})(Z_1 \otimes Z_2)' = Z_1 Z_1' \otimes Z_2 Z_2' + (Z_1 \otimes Z_2)K_{n+m}(Z_1 \otimes Z_2)'$$

$$= Z_1 Z_1' \otimes Z_2 Z_2' + K_{nm}(Z_2 \otimes Z_1)(Z_1' \otimes Z_2')$$

$$= Z_1 Z_1' \otimes Z_2 Z_2' + K_{nm}(Z_2 Z_1' \otimes Z_1 Z_2'),$$

according to Theorem 3.1 (viii). Also,

$$E(\mu_1(Z_1 w)' \otimes Z_2 w \mu_2') = E(\mu_1 \otimes (Z_1 w)' \otimes (Z_2 w) \otimes \mu_2')$$

$$= \mu_1 \otimes \left[E(Z_2 w w' Z_1') \right] \otimes \mu_2' = \mu_1 \otimes (Z_2 Z_1') \otimes \mu_2'.$$

Thus,

$$\text{Var}(x \otimes y) = Z_1 Z_1' \otimes Z_2 Z_2' + K_{nm}(Z_2 Z_1' \otimes Z_1 Z_2') + Z_1 Z_1' \otimes \mu_2 \mu_2'$$
$$+ \mu_1 \mu_1' \otimes Z_2 Z_2' + \mu_1 \otimes Z_2 Z_1' \otimes \mu_2' + \mu_1' \otimes Z_1 Z_2' \otimes \mu_2$$
$$= P \otimes R + K_{nm}(Q \otimes Q') + P \otimes \mu_2 \mu_2' + \mu_1 \mu_1' \otimes R$$
$$+ \mu_1 \otimes Q \otimes \mu_2' + \mu_1' \otimes Q' \otimes \mu_2.$$

From Theorem 3.1 (x) we see that

$$\mu_1 \otimes Q \otimes \mu_2' = K_{nm}(Q \otimes \mu_1 \mu_2')$$

and

$$\mu_1' \otimes Q' \otimes \mu_2 = K_{nm}(\mu_2 \mu_1' \otimes Q').$$

This leads to

$$\text{Var}(x \otimes y) = P \otimes R + P \otimes \mu_2 \mu_2' + \mu_1 \mu_1' \otimes R$$
$$+ K_{nm}(Q \otimes Q' + Q \otimes \mu_1 \mu_2' + \mu_2 \mu_1' \otimes Q')$$
$$= (P + \mu_1 \mu_1') \otimes (R + \mu_2 \mu_2') + K_{nm}[(Q + \mu_2 \mu_1') \otimes (Q' + \mu_1 \mu_2')]$$
$$- \mu_1 \mu_1' \otimes \mu_2 \mu_2' - K_{nm}(\mu_2 \mu_1' \otimes \mu_1 \mu_2')$$
$$= (Exx') \otimes (Eyy') + K_{nm}[(Eyx') \otimes (Exy')]$$
$$- \mu_1 \mu_1' \otimes \mu_2 \mu_2' - K_{nm}(\mu_2 \otimes \mu_1)(\mu_1' \otimes \mu_2')$$
$$= (Exx') \otimes (Eyy') + K_{nm}[(Eyx') \otimes (Exy')]$$
$$- 2\mu_1 \mu_1' \otimes \mu_2 \mu_2',$$

according to Theorem 3.1 (ix). This concludes the proof of (ii).

Further,

$$\text{tr}(\text{Var}(x \otimes y)) = (\text{tr } P)(\text{tr } R) + (\text{tr } P)(\mu_2' \mu_2) + (\mu_1' \mu_1)(\text{tr } R)$$
$$+ \text{tr } K_{nm}(Q \otimes Q') + \text{tr } K_{nm}(Q \otimes \mu_1 \mu_2') + \text{tr } K_{nm}(\mu_2 \mu_1' \otimes Q')$$
$$= (\text{tr } P)(\text{tr } R) + (\mu_2' \mu_2)\text{tr } P + (\mu_1' \mu_1)\text{tr } R$$
$$+ \text{tr}(Q'Q) + \text{tr}(\mu_1 \mu_2' Q) + \text{tr}(Q' \mu_2 \mu_1'),$$

by Theorem 3.1 (xiii). As

$$\text{tr}(\mu_1 \mu_2' Q) = \text{tr}(Q' \mu_2 \mu_1') = \mu_1' Q' \mu_2,$$

the proof of (iii) is completed. Now, let $m = n$, $\mu_1 = \mu_2 = \mu$, $P = Q = Q' = R = V$, then we find from (ii) that

$$\text{Var}(x \otimes x) = (I + K_n)(V \otimes V + V \otimes \mu\mu' + \mu\mu' \otimes V),$$

where $x \sim N(\mu, V)$.

From Theorem 3.1 (vi) we know the eigenvalues of K_n. The eigenvalues of $I + K_n$ are therefore 2 (with multiplicity $\frac{1}{2}n(n + 1)$) and 0 (with multiplicity $\frac{1}{2}n(n - 1)$). Hence, rank$(I + K_n) = \frac{1}{2}n(n + 1)$. Sufficient to show then is the non-singularity of the matrix

$$V \otimes V + V \otimes \mu\mu' + \mu\mu' \otimes V.$$

Pre- and postmultiplying with $V^{-\frac{1}{2}} \otimes V^{-\frac{1}{2}}$ we see that

$$\text{rank}(V \otimes V + V \otimes \mu\mu' + \mu\mu' \otimes V) = \text{rank}(I \otimes I + I \otimes W + W \otimes I),$$

where $W = V^{-\frac{1}{2}}\mu\mu'V^{-\frac{1}{2}}$ possesses $n - 1$ eigenvalues 0 and one eigenvalue $\alpha = \mu'V^{-1}\mu$. The distinct eigenvalues of $I \otimes W + W \otimes I$ are therefore 0, α, and 2α, and the distinct eigenvalues of $I \otimes I + I \otimes W + W \otimes I$ are 1, $1 + \alpha$, and $1 + 2\alpha$. Since $\alpha \geqslant 0$ all eigenvalues of $I \otimes I + I \otimes W + W \otimes I$ are nonzero implying its nonsingularity.

Thus $V \otimes V + V \otimes \mu\mu' + \mu\mu' \otimes V$ is nonsingular. This completes the proof.

As a final application we shall derive the variance of the (non)central Wishart distribution. Consider k statistically independent vectors $y_1, y_2, \cdots, y_k$, all of order n with

$$y_i \sim N_n(\mu_i, V) \qquad\qquad i = 1 \cdots k.$$

Define the (n, k) matrix

$$M' = (\mu_1, \mu_2, \cdots, \mu_k).$$

The joint distribution of the elements of the matrix

$$S = \sum_{i=1}^{k} y_i y_i'$$

is said to be Wishart with k degrees of freedom and is denoted by $W_n(k, V, M)$. The distribution is said to be central when $M = 0$. (See Rao (1973), page 534. Note that M instead of $M'M$ appears in the expression between brackets. The latter would seem more logical.)

The variances and covariances of the *central* Wishart distribution are given element by element in Anderson (1958, page 161). The following theorem gives the complete covariance matrix for a (noncentrally) Wishart distributed stochastic matrix.

THEOREM 4.4.   *Let S be Wishart distributed $W_n(k, V, M)$, V positive definite, then*

(i) $ES = kV + M'M$,

(ii) $\text{Var}(\text{vec } S) = (I + K_n)[k(V \otimes V) + V \otimes (M'M) + (M'M) \otimes V]$.

PROOF.

$$ES = E\sum_i y_i y_i' = \sum_i E y_i y_i' = \sum_i (V + \mu_i \mu_i') = kV + M'M.$$

$\text{Var}(\text{vec } S) = \text{Var}(\text{vec } \sum_i y_i y_i') = \text{Var}(\sum_i \text{vec } y_i y_i') = \sum_i \text{Var}(\text{vec } y_i y_i') = \sum_i \text{Var}(y_i \otimes y_i).$

From Theorem 4.3 (iv) we know that

$$\text{Var}(y_i \otimes y_i) = (I + K_n)(V \otimes V + V \otimes \mu_i \mu_i' + \mu_i \mu_i' \otimes V).$$

Thus,

$$\text{Var}(\text{vec } S) = \sum_i (I + K_n)(V \otimes V + V \otimes \mu_i \mu_i' + \mu_i \mu_i' \otimes V)$$

$$= (I + K_n)\left[k(V \otimes V) + V \otimes (\sum_i \mu_i \mu_i') + (\sum_i \mu_i \mu_i') \otimes V \right]$$

$$= (I + K_n)\left[k(V \otimes V) + V \otimes (M'M) + (M'M) \otimes V \right].$$

A special case is the central Wishart distribution, where $M = 0$.

COROLLARY 4.2. *Let S be centrally Wishart distributed* $W_n(k, V)$, *then*

$$ES = kV$$
$$\text{Var}(\text{vec } S) = k(I + K_n)(V \otimes V).$$

Another special case arises when we put $n = 1$:

COROLLARY 4.3. *Let* $x_i \sim N(\mu_i, 1)$, $(i = 1 \cdots k)$ *be independent variables. Then* $x = \sum_i x_i^2$ *is said to be noncentrally* χ^2 *distributed with* k *degrees of freedom and noncentrality parameter* $\lambda = \sum_i \mu_i^2$. *We have*

$$Ex = k + \lambda$$
$$\text{Var}(x) = 2k + 4\lambda,$$

which includes the central χ^2 *(where* $\lambda = 0$*) as a special case.*

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