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HADAMARD, KHATRI-RAO, KRONECKER AND OTHER MATRIX PRODUCTS

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This paper is dedicated to Heinz Neudecker, with affection and appreciation

Abstract. In this paper we present a brief overview on Hadamard, Khatri-Rao, Kronecker and several related non-simple matrix products and their properties. We include practical applications, in different areas, of some of the algebraic results.

Key Words. Hadamard (or Schur) product, Khatri-Rao product, Tracy-Singh product, Kronecker product, vector cross product, positive definite variance matrix, multi-way model, linear matrix equation, signal processing.

1. Introduction

Matrices and matrix operations are studied and applied in many areas such as engineering, natural and social sciences. Books written on these topics include Berman et al. (1989), Barnett (1990), Lütkepohl (1996), Schott (1997), Magnus and Neudecker (1999), Hogben (2006), Schmidt and Trenkler (2006), and especially Bernstein (2005) with a number of referred books classified as for different areas in the preface. In this paper, we will in particular overview briefly results (with practical applications) involving several non-simple matrix products, as they play a very important role nowadays and deserve to receive such attention.

The Hadamard (or Schur) and Kronecker products are studied and applied widely in matrix theory, statistics, system theory and other areas; see, e.g. Styan (1973), Neudecker and Liu (1995), Neudecker and Satorra (1995), Trenkler (1995), Rao and Rao (1998), Zhang (1999), Liu (2000a, 2000b) and Van Trees (2002). Horn (1990) presents an excellent survey focusing on the Hadamard product. Magnus and Neudecker (1999) include basic results and statistical applications involving Hadamard or Kronecker products. An equality connection between the Hadamard and Kronecker products seems to be firstly used by e.g. Browne (1974), Pukelsheim (1977) and Faliva (1983). Trenkler (2001, 2002) and Neudecker and Trenkler (2005, 2006a) study the Kronecker and vector cross products.

For partitioned matrices, the Khatri-Rao product, viewed as a generalized Hadamard product, is discussed and used by e.g. Khatri and Rao (1968), Rao (1970), Rao and Kleffe (1988), Horn and Mathias (1992), Liu (1995, 1999, 2002a), Rao and Rao (1998), and Yang (2002a, 2002b, 2003, 2005) and his co-authors. The Tracy-Singh product, as a generalized Kronecker product, is studied by e.g. Singh

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(1972), Tracy and Singh (1972), Hyland and Collins (1989), Tracy and Jinadasa (1989) and Koning et al. (1991). A connection between the Khatri-Rao and Tracy-Singh products and several results involving these two products of positive definite matrices with statistical applications are given by Liu (1999).

In the present paper, we make an attempt to provide a brief overview on some selected results recently obtained on the Hadamard, Khatri-Rao, Kronecker and other products, and do not intend to present a complete list of all the existing results. We stress that the Khatri-Rao product has significant applications and potential in many areas, including matrices, mathematics, statistics (including psychometrics and econometrics), and signal processing systems. Further attention and studies on the Khatri-Rao product will prove to be useful. In Section 2, we introduce the definitions of the Hadamard, Kronecker, Khatri-Rao, Tracy-Singh and vector cross products, and the Khatri-Rao and Tracy-Singh sums, with basic relations among the products. In Section 3, we present some equalities and inequalities involving positive definite matrices. We collect both well-known and existing but not widely-known inequalities involving the Hadamard product; on the other hand, the results can not be extended to cover the Khatri-Rao product. We collect several known inequalities involving the Khatri-Rao product and results involving the Kronecker and vector cross products, including those to be used in Section 4. Finally we compile some applications of the results involving the Khatri-Rao product, as examples to illustrate how the results can be used in various areas.

2. Basic results

We give the definitions of these matrix products and established relations among them. We deal with only real matrices in this paper.

2.1. Definitions. Consider matrices $\mathbf{A} = (a_{ij})$ and $\mathbf{C} = (c_{ij})$ of order $m \times n$ and $\mathbf{B} = (b_{kl})$ of order $p \times q$. Let $\mathbf{A} = (\mathbf{A}_{ij})$ be partitioned with $\mathbf{A}_{ij}$ of order $m_i \times n_j$ as the (i, j)th block submatrix and $\mathbf{B} = (\mathbf{B}_{kl})$ be partitioned with $\mathbf{B}_{kl}$ of order $p_k \times q_l$ as the (k, l)th block submatrix ($\sum m_i = m$, $\sum n_j = n$, $\sum p_k = p$ and $\sum q_l = q$). The definitions of the matrix products or sums of $\mathbf{A}$ and $\mathbf{B}$ are given as follows.

2.1.1. Hadamard product.

$$\mathbf{A} \odot \mathbf{C} = (a_{ij} c_{ij})_{ij}, \tag{1}$$

where $a_{ij} c_{ij}$ is a scalar and $\mathbf{A} \odot \mathbf{C}$ is of order $m \times n$.

2.1.2. Kronecker product.

$$\mathbf{A} \otimes \mathbf{B} = (a_{ij} \mathbf{B})_{ij}, \tag{2}$$

where $a_{ij} \mathbf{B}$ is of order $p \times q$ and $\mathbf{A} \otimes \mathbf{B}$ is of order $mp \times nq$.

2.1.3. Khatri-Rao product.

$$\mathbf{A} * \mathbf{B} = (\mathbf{A}_{ij} \otimes \mathbf{B}_{ij})_{ij}, \tag{3}$$

where $\mathbf{A}_{ij} \otimes \mathbf{B}_{ij}$ is of order $m_i p_i \times n_j q_j$ and $\mathbf{A} * \mathbf{B}$ is of order $(\sum m_i p_i) \times (\sum n_j q_j)$.

2.1.4. Tracy-Singh product.

$$\mathbf{A} \bowtie \mathbf{B} \quad = \quad (\mathbf{A}_{ij} \bowtie \mathbf{B})_{ij} = ((\mathbf{A}_{ij} \otimes \mathbf{B}_{kl})_{kl})_{ij}, \tag{4}$$

where $\mathbf{A}_{ij} \otimes \mathbf{B}_{kl}$ is of order $m_i p_k \times n_j q_l$, $\mathbf{A}_{ij} \bowtie \mathbf{B}$ is of order $m_i p \times n_j q$ and $\mathbf{A} \bowtie \mathbf{B}$ is of order $mp \times nq$.

2.1.5. Khatri-Rao sum.

$$\mathbf{A} \diamond \mathbf{B} = \mathbf{A} * \mathbf{I}_p + \mathbf{I}_m * \mathbf{B}, \tag{5}$$

where $\mathbf{A} = (\mathbf{A}_{ij})$ and $\mathbf{B} = (\mathbf{B}_{kl})$ are square matrices of respective order $m \times m$ and $p \times p$ with $\mathbf{A}_{ij}$ of order $m_i \times m_j$ and $\mathbf{B}_{kl}$ of order $p_k \times p_l$, $\mathbf{I}_p$ and $\mathbf{I}_m$ are compatibly partitioned identity matrices, and $\mathbf{A} \diamond \mathbf{B}$ is of order $(\sum m_i p_i) \times (\sum m_i p_i)$.

2.1.6. Tracy-Singh sum.

$$\mathbf{A} \Box \mathbf{B} \quad = \quad \mathbf{A} \bowtie \mathbf{I}_p + \mathbf{I}_m \bowtie \mathbf{B}, \tag{6}$$

where $\mathbf{A} = (\mathbf{A}_{ij})$ and $\mathbf{B} = (\mathbf{B}_{kl})$ are square matrices of respective order $m \times m$ and $p \times p$ with $\mathbf{A}_{ij}$ of order $m_i \times m_j$ and $\mathbf{B}_{kl}$ of order $p_k \times p_l$, $\mathbf{I}_p$ and $\mathbf{I}_m$ are compatibly partitioned identity matrices, and $\mathbf{A} \Box \mathbf{B}$ is of order $mp \times mp$.

2.1.7. Vector cross product.

$$\mathbf{a} \times \mathbf{b} = \mathbf{T}_{\mathbf{a}} \mathbf{b}, \tag{7}$$

where $\mathbf{a} = (a_1, a_2, a_3)'$ and $\mathbf{b} = (b_1, b_2, b_3)'$ are real vectors, and

$$\mathbf{T}_{\mathbf{a}} = \begin{pmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{pmatrix}.$$

For (1) through (4) see e.g. Liu (1999). For (3) introduced in the column-wise partitioned case, see Khatri and Rao (1968) and Rao and Rao (1998). For (5) and (6) see Al Zhour and Kilicman (2006b). For (7), see Trenkler (1998, 2001, 2002) and Neudecker and Trenkler (2005, 2006a).

Note that there are various different names and symbols used in the literature for the five products mentioned above; e.g. block Kronecker products by Koning et al. (1991) and Horn and Mathias (1992), in addition to some other matrix products. In particular, the Tracy-Singh product is the same as one of the block Kronecker products and the Hadamard product is the Schur product. Further, the Khatri-Rao and Tracy-Singh products share some similarities with, but also are quite different from, the Hadamard and Kronecker products, respectively. Certainly the connections and differences need attention, and we refer these to e.g. Koning et al. (1991), Horn and Mathias (1992), Wei and Zhang (2000) and Yang (2003, 2005) regarding matrix sizes, partitions and operational properties for these matrix products. In the next subsection, we report some relations connecting the products.

2.2. Relations.

2.2.1. Hadamard and Kronecker products. It is known that the Hadamard product of two matrices is the principal submatrix of the Kronecker product of the two matrices. This relation can be expressed in an equation as follows.

Lemma 1. *For* $\mathbf{A}$ *and* $\mathbf{C}$ *of the same order* $m \times n$ *we have*

$$\mathbf{A} \odot \mathbf{C} = \mathbf{J}_1'(\mathbf{A} \otimes \mathbf{C})\mathbf{J}_2, \tag{8}$$

where $\mathbf{J}_1$ *is the selection matrix of order* $m^2 \times m$ *and* $\mathbf{J}_2$ *is the selection matrix of order* $n^2 \times n$.

For this relation, see e.g. Faliva (1983) and Liu (1999). For $\mathbf{J}$ with properties including $\mathbf{J}'\mathbf{J} = \mathbf{I}$ and applications, see e.g. Browne (1974), Pukelsheim (1977), Liu (1995), Liu and Neudecker (1996), Neudecker et al. (1995a, b), Neudecker and Liu (2001a, b) and Schott (1997, p. 267). We next present the relation between Khatri-Rao and Tracy-Singh products which extends the above.

2.2.2. Khatri-Rao and Tracy-Singh products. Without loss of generality, we consider here 2×2 block matrices

$$\mathbf{A} = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{pmatrix}, \tag{9}$$

where $\mathbf{A}$, $\mathbf{A}_{11}$, $\mathbf{A}_{12}$, $\mathbf{A}_{21}$, $\mathbf{A}_{22}$, $\mathbf{B}$, $\mathbf{B}_{11}$, $\mathbf{B}_{12}$, $\mathbf{B}_{21}$ and $\mathbf{B}_{22}$ are $m \times n$, $m_1 \times n_1$, $m_1 \times n_2$, $m_2 \times n_1$, $m_2 \times n_2$, $p \times q$, $p_1 \times q_1$, $p_1 \times q_2$, $p_2 \times q_1$ and $p_2 \times q_2$ ($m_1 + m_2 = m$, $n_1 + n_2 = n$, $p_1 + p_2 = p$ and $q_1 + q_2 = q$) matrices respectively.

Further,

$$\mathbf{M} = \begin{pmatrix} \mathbf{M}_{11} & \mathbf{M}_{12} \\ \mathbf{M}'_{12} & \mathbf{M}_{22} \end{pmatrix}, \quad \mathbf{N} = \begin{pmatrix} \mathbf{N}_{11} & \mathbf{N}_{12} \\ \mathbf{N}'_{12} & \mathbf{N}_{22} \end{pmatrix}, \tag{10}$$

where $\mathbf{M}$, $\mathbf{M}_{11}$, $\mathbf{M}_{22}$, $\mathbf{N}$, $\mathbf{N}_{11}$ and $\mathbf{N}_{22}$ are $m \times m$, $m_1 \times m_1$, $m_2 \times m_2$, $p \times p$, $p_1 \times p_1$ and $p_2 \times p_2$ symmetric matrices respectively, and $\mathbf{M}_{12}$ and $\mathbf{N}_{12}$ are $m_1 \times m_2$ and $p_1 \times p_2$ matrices respectively.

Define the following selection matrices $\mathbf{Z}_1$ of order $k_1 \times r$ and $\mathbf{Z}_2$ of order $k_2 \times s$:

$$\mathbf{Z}_1 = \begin{pmatrix} \mathbf{I}_{11} & \mathbf{0}_{11} & \mathbf{0}_{21} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I}_{21} \end{pmatrix}', \quad \mathbf{Z}_2 = \begin{pmatrix} \mathbf{I}_{12} & \mathbf{0}_{12} & \mathbf{0}_{22} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I}_{22} \end{pmatrix}', \tag{11}$$

where $\mathbf{Z}'_1\mathbf{Z}_1 = \mathbf{I}_1$ and $\mathbf{Z}'_2\mathbf{Z}_2 = \mathbf{I}_2$ with $\mathbf{I}_{11}, \mathbf{I}_{21}, \mathbf{I}_{12}, \mathbf{I}_{22}, \mathbf{I}_1$ and $\mathbf{I}_2$ being $m_1p_1 \times m_1p_1$, $m_2p_2 \times m_2p_2$, $n_1q_1 \times n_1q_1$, $n_2q_2 \times n_2q_2$, $r \times r$ and $s \times s$ identity matrices ($k_1 = mp$, $k_2 = nq$, $m = m_1 + m_2$, $n = n_1 + n_2$, $p = p_1 + p_2$, $q = q_1 + q_2$, $r = m_1p_1 + m_2p_2$ and $s = n_1q_1 + n_2q_2$), and $\mathbf{0}_{11}$, $\mathbf{0}_{21}$, $\mathbf{0}_{12}$ and $\mathbf{0}_{22}$ being $m_1p_1 \times m_1p_2$, $m_1p_1 \times m_2p_1$, $n_1q_1 \times n_1q_2$ and $n_1q_1 \times n_2q_1$ matrices of zeros.

In particular, if $k = k_i$, $m_i = n_i$ and $p_i = q_i$, $i = 1, 2$ in (11), we have

$$\mathbf{Z} = \mathbf{Z}_1 = \mathbf{Z}_2, \tag{12}$$

where $\mathbf{Z}$ is the $k \times r$ selection matrix such that $\mathbf{Z}'\mathbf{Z} = \mathbf{I}$.

Lemma 2. *For* $\mathbf{A}$ *and* $\mathbf{B}$ *partitioned as in (9) and* $\mathbf{M}$ *and* $\mathbf{N}$ *partitioned as in (10), we have*

$$\mathbf{A} * \mathbf{B} = \mathbf{Z}'_1(\mathbf{A} \bowtie \mathbf{B})\mathbf{Z}_2, \tag{13}$$

$$\mathbf{M} * \mathbf{N} = \mathbf{Z}'(\mathbf{M} \bowtie \mathbf{N})\mathbf{Z}. \tag{14}$$

Note that the basic idea for (13) and (14) in the above-mentioned case for 2×2 block matrices $\mathbf{A}$ and $\mathbf{B}$ can be generalised to a multiple case for $s \times t$ block matrices $\mathbf{A} = (\mathbf{A}_{ij})$ and $\mathbf{B}$ where $i = 1, \ldots, s$, $j = 1, \ldots, t$ and s, $t > 2$; see e.g. Cao et al. (2002) and Yang (2002b). Further, the symmetric partition of square matrices with $s = t > 2$, considered as in e.g. Koning et al. (1991), Horn and Mathias (1992) and Wei and Zhang (2000) are particularly useful. Clearly $\mathbf{M}$ and $\mathbf{N}$ in (10) for which (14) holds can be partitioned as $s \times s$ block matrices, $s > 2$, and corresponding results involving $\mathbf{M}$ and $\mathbf{N}$ can be given. To study results involving the Khatri-Rao product generalised from those involving the Hadamard product, it is convenient to consider $s > 2$.

2.2.3. Tracy-Singh and Kronecker products. The following is well established.

Lemma 3. *For the Tracy-Singh and Kronecker products, we have*

$$\mathbf{A} \bowtie \mathbf{B} = \mathbf{P}_1'(\mathbf{A} \otimes \mathbf{B})\mathbf{P}_2, \tag{15}$$

where $\mathbf{P}_i$ $(i = 1, 2)$ *is a permutation matrix.*

This result has been given independently; see e.g. Koning et al. (1991), Horn and Mathias (1992) and Wei and Zhang (2000).

2.2.4. Khatri-Rao and Kronecker products. The following is a consequence of Lemma 3.

Lemma 4. *For the Khatri-Rao and Kronecker products, we have*

$$\mathbf{A} * \mathbf{B} \quad = \quad \mathbf{Q}_1'(\mathbf{A} \otimes \mathbf{B})\mathbf{Q}_2, \tag{16}$$

where $\mathbf{Q}_i$ *is a selection matrix such that* $\mathbf{Q}_i = \mathbf{P}_i\mathbf{Z}_i$*,* $\mathbf{P}_i$ *is as in Lemma 3 and* $\mathbf{Z}_i$ *is as in Lemma 2* $(i = 1, 2)$*.*

2.2.5. Column-wise partitioned case. As a special case, we consider $\mathbf{A}$ and $\mathbf{B}$ with the same number of columns but not necessarily the same number of rows; i.e., $\mathbf{A} = (\mathbf{a}_1, \dots, \mathbf{a}_n)$ and $\mathbf{B} = (\mathbf{b}_1, \dots, \mathbf{b}_n)$, where $\mathbf{a}_i$ and $\mathbf{b}_i$ are the ith columns of $\mathbf{A}$ and $\mathbf{B}$ respectively, $i = 1, \dots, n$.

$$\mathbf{A} * \mathbf{B} \quad = \quad (\mathbf{A} \bowtie \mathbf{B})\mathbf{Z}_2, \tag{17}$$

$$\mathbf{J}_1'(\mathbf{A} * \mathbf{C}) \quad = \quad (\mathbf{A} \odot \mathbf{C}),\ \text{for } \mathbf{A} \text{ and } \mathbf{C} \text{ of the same size} \tag{18}$$

where $\mathbf{Z}_2$ is the same as above, $\mathbf{J}_1 = (\mathbf{e}_1, \dots, \mathbf{e}_n)'$ is an $n^2 \times n$ selection matrix and $\mathbf{e}_i$ is the ith unit vector, $i = 1, \dots, n$. When the Kronecker product is considered, instead of the Khatri-Rao product in (17), as a special case we have

$$\mathbf{A} * \mathbf{B} = (\mathbf{A} \otimes \mathbf{B})\mathbf{J}_2. \tag{19}$$

For its applications, see e.g. Lev-Ari (2005).

2.2.6. Kronecker and vector cross products. There is a close connection between the vector cross product and the Kronecker product; see Trenkler (2001). Define

$$\begin{aligned}
\mathbf{E}_1 \quad &= \quad (\mathbf{e}_2\mathbf{e}_1' + \mathbf{e}_3\mathbf{e}_2',\ \mathbf{e}_3\mathbf{e}_3' - \mathbf{e}_1\mathbf{e}_1',\ -\mathbf{e}_1\mathbf{e}_2' - \mathbf{e}_2\mathbf{e}_3'), \\
\mathbf{E}_2 \quad &= \quad \mathbf{e}_1\mathbf{e}_3' - \mathbf{e}_2\mathbf{e}_2' + \mathbf{e}_3\mathbf{e}_1',
\end{aligned}$$

where $\mathbf{e}_i$ is a 3×1 unit vector, $\mathbf{E}_1$ is a 3×9 matrix and $\mathbf{E}_2$ is a 3×3 matrix. Then

$$\mathbf{a} \times \mathbf{b} = \mathbf{E}_1(\mathbf{I}_3 \otimes \mathbf{E}_2)(\mathbf{b} \otimes \mathbf{a}) = \mathbf{E}_1(\mathbf{b} \otimes \mathbf{E}_2\mathbf{a}) \tag{20}$$

or alternatively

$$\mathbf{a} \times \mathbf{b} = -\mathbf{E}_1(\mathbf{I}_3 \otimes \mathbf{E}_2)(\mathbf{a} \otimes \mathbf{b}) = -\mathbf{E}_1(\mathbf{a} \otimes \mathbf{E}_2\mathbf{b}).$$

We will next consider some equalities and inequalities. Hereafter, we write $\mathbf{M} \geq \mathbf{P}$ in the *Löwner* ordering sense meaning that $\mathbf{M} - \mathbf{P} \geq 0$ is non-negative definite, for symmetric matrices $\mathbf{M}$ and $\mathbf{P}$ of the same order. Let $()^+$ indicate the Moore-Penrose inverse of the matrix. Denote $\mathbf{H}^0 = \mathbf{H}\mathbf{H}^+$, for $\mathbf{H}$ a non-negative definite matrix.

3. Equalities and inequalities

Here we select some equalities and inequalities. For further results, see the references cited afterwards.

3.1. Equalities. We select three simple but important results.

Theorem 1. *For* $\mathbf{A}$, $\mathbf{B}$, $\mathbf{D}$ *and* $\mathbf{E}$ *compatibly partitioned, we have*

$$(\mathbf{A}+\mathbf{B})*\mathbf{D} = \mathbf{A}*\mathbf{D}+\mathbf{B}*\mathbf{D}, \tag{21}$$

$$(\mathbf{A}*\mathbf{B})*\mathbf{D} = \mathbf{A}*(\mathbf{B}*\mathbf{D}), \tag{22}$$

$$(\mathbf{A}*\mathbf{B})\odot(\mathbf{D}*\mathbf{E}) = (\mathbf{A}\odot\mathbf{D})*(\mathbf{B}\odot\mathbf{E}). \tag{23}$$

See e.g. Liu (1999).

Theorem 2. *For the column-wise partitioned case,*

$$(\mathbf{C}\otimes\mathbf{D})(\mathbf{A}*\mathbf{B}) = \mathbf{CA}*\mathbf{DB} \tag{24}$$

$$(\mathbf{A}*\mathbf{B})'(\mathbf{A}*\mathbf{B}) = \mathbf{A}'\mathbf{A}\odot\mathbf{B}'\mathbf{B}, \tag{25}$$

$$(\mathbf{A}*\mathbf{B})^+ = [(\mathbf{A}'\mathbf{A})\odot(\mathbf{B}'\mathbf{B})]^+(\mathbf{A}*\mathbf{B})', \tag{26}$$

$$\mathrm{vec}(\mathbf{AXB}) = (\mathbf{B}'\otimes\mathbf{A})\,\mathrm{vec}(\mathbf{X}) = (\mathbf{B}'*\mathbf{A})\,\mathrm{vecd}(\mathbf{X}), \tag{27}$$

where vec *denotes the vectorization operator which transforms a matrix into a vector by stacking the columns of the matrix one underneath the other,* vecd *indicates the vectorization operator which selects only the diagonal elements of the matrix into a vector, and the Moore-Penrose inverse in (26) becomes the ordinary inverse when both* $\mathbf{A}$ *and* $\mathbf{B}$ *are of full column rank.*

For (24) and (25), see e.g. Rao and Rao (1998). For (25), see also Bro (1998). For (26) and (27), see e.g. Lev-Ari (2005).

3.2. Inequalities involving Hadamard product. The results presented here should be useful.

Theorem 3. *For* $n \times n$ *positive definite matrices* A *and* D, *and* $n \times n$ *positive definite correlation matrices* B *and* C, *we have*

$$\mathbf{I} \leq \mathbf{A}\odot\mathbf{A}^{-1} \leq \frac{\lambda^2+\mu^2}{2\lambda\mu}\,\mathbf{I}, \tag{28}$$

$$\frac{2\lambda^{1/2}\mu^{1/2}}{\lambda+\mu}\,\mathbf{I} \leq \mathbf{B}^{1/2}\odot\mathbf{C}^{1/2} \leq \mathbf{I}, \tag{29}$$

$$2\,\mathrm{tr}(\mathbf{A}\odot\mathbf{D}) \leq \mathrm{tr}(\mathbf{A}\odot\mathbf{A}+\mathbf{D}\odot\mathbf{D}), \tag{30}$$

where $\mathbf{I}$ *is the* $n\times n$ *identity matrix, and* λ *and* μ *are positive numbers such that the eigenvalues of* $\mathbf{A}$, $\mathbf{B}$ *and* $\mathbf{C}$ *are contained in the interval* $[\lambda, \mu]$.

For the first relationship in (28) and its applications see e.g. Horn (1990) and Schott (1997, pp. 275-276), and for the second see Liu (1995). For an extension with more items added into the middle of the inequalities (28), see e.g. Bernstein (2005, pp. 333-341). For the second relationship in (29) see Zhang (2000), and for the first see Liu (2002b, 2003). For (30), see Neudecker and Liu (1993). For more results and applications involving the Hadamard product, see e.g. Styan (1973), Visick (1990, 1998, 2000), Neudecker et al. (1995), Zhang (1999) and Liu (2000a, 2000b, 2001).

3.3. Inequalities involving Kronecker product. The Kronecker product is the most widely used. We present an elegant result.

Theorem 4. *For non-negative matrices* $\mathbf{A}$ *and* $\mathbf{B}$ *we have*

$$\mathbf{A} \otimes \mathbf{A} \geq \mathbf{B} \otimes \mathbf{B} \text{ is equivalent to } \mathbf{A} \geq \mathbf{B}. \tag{31}$$

This is established as an Econometric Theory problem and solution; see Neudecker and Satorra (1995) with the sufficient condition, Trenkler (1995) with the necessary and sufficient condition using a result given by Baksalary et al. (1992), and Neudecker and Liu (1995) with the necessary condition. A special case is $\mathbf{A} = E(\mathbf{z}\mathbf{z}')$, $\mathbf{B} = (E\mathbf{z})(E\mathbf{z})'$ and $\mathbf{A} - \mathbf{B} = D(\mathbf{z})$, where E and D denote expected value and covariance matrix, respectively, of a random variable $\mathbf{z}$. Note that if we consider only the sufficient condition, the inequality still holds when the Kronecker product is replaced by the Hadamard product. For both results involving the two products, see e.g. Bernstein (2005, p. 336).

The Kronecker product has been studied by Neudecker (1969), has been covered by two reviews (Henderson and Searle (1979, 1981)), is involved in Jacobian matrices and matrix calculus (Mathai (1997) and Magnus and Neudecker (1999)), and is very recently used by several authors (see e.g. Bernstein (2005), Neudecker (2006), Neudecker and Trenkler (2006b), and Schmidt and Trenkler (2006)).

3.4. Inequalities involving Khatri-Rao product. We select the following inequalities.

Theorem 5. *Let* $\mathbf{A}$ *and* $\mathbf{B}$ *be partitioned as in (1). Then*

$$\mathbf{A}'\mathbf{A} * \mathbf{B}'\mathbf{B} \geq (\mathbf{A}' * \mathbf{B}')(\mathbf{A} * \mathbf{B}). \tag{32}$$

This extends a result involving the Hadamard product, which can be found in Amemiya (1985).

Theorem 6. *Let* $\mathbf{M} \geq \mathbf{P} \geq \mathbf{0}$, $\mathbf{N} \geq \mathbf{Q} \geq \mathbf{0}$, *and* $\mathbf{M}$, $\mathbf{P}$, $\mathbf{N}$ *and* $\mathbf{Q}$ *be compatibly partitioned matrices. Then*

$$\mathbf{M} * \mathbf{N} \geq \mathbf{P} * \mathbf{Q} \geq \mathbf{0}. \tag{33}$$

Let $\mathbf{M}$ *be partitioned as in (2) with* $\mathbf{M}_{11} \geq \mathbf{0}$ *and* $\mathbf{M}_{22} \geq \mathbf{0}$. *Then*

$$\mathbf{M} * \mathbf{M} \geq \mathbf{0} \text{ is equivalent to } \mathbf{M} \geq \mathbf{0}. \tag{34}$$

Let $\mathbf{M} \geq \mathbf{0}$ *such that* $\mathbf{M}_{11} > \mathbf{0}$ *and* $\mathbf{M}_{22} > \mathbf{0}$. *Then*

$$\mathbf{N} > \mathbf{0} \text{ implies } \mathbf{M} * \mathbf{N} > \mathbf{0}. \tag{35}$$

If $\mathbf{M} \geq \mathbf{0}$ *and* $\mathbf{M}_{11} = \mathbf{M}_{12} = \mathbf{M}_{22}$, *then*

$$\mathbf{M} * \mathbf{N} > \mathbf{0} \text{ is equivalent to } \mathbf{M}_{11} > \mathbf{0} \text{ and } \mathbf{N} > \mathbf{0}. \tag{36}$$

Theorem 7. *Let* $\mathbf{M} > \mathbf{0}$ *and* $\mathbf{N} > \mathbf{0}$ *be* $m \times m$ *and* $p \times p$ *positive definite matrices partitioned as in (2),* $\mathbf{I}$ *an* $r \times r$ *identity matrix,* $r = m_1p_1 + m_2p_2$, $m = m_1 + m_2$,

$p = p_1 + p_2$ and $k = mp$. Then

$$(\mathbf{M} * \mathbf{N})^{-1} \leq \mathbf{M}^{-1} * \mathbf{N}^{-1}; \tag{37}$$

$$\mathbf{M}^{-1} * \mathbf{N}^{-1} \leq \frac{(\lambda_1 + \lambda_k)^2}{4\lambda_1\lambda_k}(\mathbf{M} * \mathbf{N})^{-1}; \tag{38}$$

$$\mathbf{M} * \mathbf{N} - (\mathbf{M}^{-1} * \mathbf{N}^{-1})^{-1} \leq (\sqrt{\lambda_1} - \sqrt{\lambda_k})^2\mathbf{I}; \tag{39}$$

$$(\mathbf{M} * \mathbf{N})^2 \leq \mathbf{M}^2 * \mathbf{N}^2; \tag{40}$$

$$\mathbf{M}^2 * \mathbf{N}^2 \leq \frac{(\lambda_1 + \lambda_k)^2}{4\lambda_1\lambda_k}.(\mathbf{M} * \mathbf{N})^2; \tag{41}$$

$$(\mathbf{M} * \mathbf{N})^2 - \mathbf{M}^2 * \mathbf{N}^2 \leq \frac{1}{4}(\lambda_1 - \lambda_k)^2\mathbf{I}; \tag{42}$$

$$\mathbf{M} * \mathbf{N} \leq (\mathbf{M}^2 * \mathbf{N}^2)^{1/2}; \tag{43}$$

$$(\mathbf{M}^2 * \mathbf{N}^2)^{1/2} \leq \frac{\lambda_1 + \lambda_k}{2\sqrt{\lambda_1\lambda_k}}\mathbf{M} * \mathbf{N}; \tag{44}$$

$$(\mathbf{M}^2 * \mathbf{N}^2)^{1/2} - \mathbf{M} * \mathbf{N} \leq \frac{(\lambda_1 - \lambda_k)^2}{4(\lambda_1 + \lambda_k)}\,\mathbf{I}, \tag{45}$$

where $\lambda_1 \geq \cdots \geq \lambda_k$ are the eigenvalues of $\mathbf{M} \bowtie \mathbf{N}$ of order $k \times k$.

For Theorems 5 through 7, see Liu (1999); Albert's theorem (see e.g. Albert (1969) and Bekker and Neudecker (1989)) plays a role in the proof. A number of studies on extensions and further related results including necessary and sufficient conditions for some inequalities to become equalities have already been made; see e.g. Brualdi (1999), Yang (2002b, 2005), Feng and Yang (2002), Han and Liu (2002), Liu (2002a, 2002b), Yang et al. (2002), Zhang et al. (2002a, 2002b), Civciv and Türkmen (2005) and Al Zhour and Kilicman (2006a, 2006b).

3.5. Results involving Schur complement. Consider positive definite matrices $\mathbf{A}$ of size $m \times m$ and $\mathbf{B}$ of size $p \times p$. Let $\mathbf{A}(\alpha, \beta)$ denote a sub-matrix of α rows and β columns taken from $\mathbf{A}$ and $\mathbf{A}(\alpha, \alpha) = \mathbf{A}(\alpha)$. Assume that $|\alpha_1| = k$, $|\alpha_2| = s$, $\alpha_1' = \{1, \ldots, m\} - \alpha_1$, $\alpha_2' = \{1, \ldots, p\} - \alpha_2$, and

$$\mathbf{A} = \begin{pmatrix} \mathbf{A}(\alpha_1) & \mathbf{A}(\alpha_1, \alpha_1') \\ \mathbf{A}(\alpha_1, \alpha_1')' & \mathbf{A}(\alpha_1') \end{pmatrix}, \tag{46}$$

$$\mathbf{B} = \begin{pmatrix} \mathbf{B}(\alpha_2) & \mathbf{B}(\alpha_2, \alpha_2') \\ \mathbf{B}(\alpha_2, \alpha_2')' & \mathbf{B}(\alpha_2') \end{pmatrix}. \tag{47}$$

For non-singular $\mathbf{A}(\alpha_1)$, its Schur complement is defined as $\mathbf{A}/\alpha_1 = \mathbf{A}(\alpha_1') - \mathbf{A}(\alpha_1', \alpha_1)\mathbf{A}(\alpha_1)^{-1}\mathbf{A}(\alpha_1, \alpha_1')$.

Theorem 8.

$$\begin{aligned} (\mathbf{A} * \mathbf{B})^{-1}/(\alpha_1 \otimes \alpha_2) &\leq [(\mathbf{A} * \mathbf{B})/(\alpha_1 \otimes \alpha_2)]^{-1} \\ &\leq (\mathbf{A}^{-1} * \mathbf{B}^{-1})/(\alpha_1 \otimes \alpha_2) \\ &\leq (\mathbf{A}/\alpha_1)^{-1} \otimes (\mathbf{B}/\alpha_2)^{-1}. \end{aligned} \tag{48}$$

For these inequalities with necessary and sufficient conditions for them to become tight, see Yang and Feng (2000). For further considerations, extensions and related results, see Yang (2002a, 2003) and Zhou and Wang (2006). In particular, a chain inequality involving principal and complementary sub-matrices which elegantly sharpens (37) is given by Yang (2003). For a general introduction to the Schur complement and collection of recent work and applications, see Zhang (2005).

3.6. Results involving Tracy-Singh product. The two results given here correspond to the results involving the Khatri-Rao product.

Theorem 9. *For* $\mathbf{A}$, $\mathbf{B}$, $\mathbf{D}$ *and* $\mathbf{E}$ *compatibly partitioned, we have*

$$(\mathbf{A} \bowtie \mathbf{B})(\mathbf{D} \bowtie \mathbf{E}) = (\mathbf{AD}) \bowtie (\mathbf{BE}), \tag{49}$$

$$(\mathbf{A} \bowtie \mathbf{B})^{+} = \mathbf{A}^{+} \bowtie \mathbf{B}^{+} \text{ for the Moore-Penrose inverse.} \tag{50}$$

Theorem 10. *Let* $\mathbf{M} \geq \mathbf{P} \geq \mathbf{0}$*,* $\mathbf{N} \geq \mathbf{Q} \geq \mathbf{0}$*, and* $\mathbf{M}$*,* $\mathbf{P}$*,* $\mathbf{N}$ *and* $\mathbf{Q}$ *be compatibly partitioned matrices. Then*

$$\mathbf{M} \bowtie \mathbf{N} \geq \mathbf{P} \bowtie \mathbf{Q} \geq \mathbf{0}, \tag{51}$$

$$\mathbf{M} \bowtie \mathbf{M} \geq \mathbf{P} \bowtie \mathbf{P} \text{ is equivalent to } \mathbf{M} \geq \mathbf{P}. \tag{52}$$

The last one corresponds to (31) for the Kronecker product. See e.g. Liu (1999).

3.7. Results involving vector cross product. Let again $\mathbf{a} = (a_1, a_2, a_3)'$ and $\mathbf{b} = (b_1, b_2, b_3)'$ be real vectors. Then

$$\mathbf{a} \times \mathbf{b} = \mathbf{T_a b}, \tag{53}$$

where

$$\mathbf{T_a} = \begin{pmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{pmatrix}.$$

The matrix $\mathbf{T_a}$ can be written as

$$\mathbf{T_a} = a_3(\mathbf{e}_2\mathbf{e}_1' - \mathbf{e}_1\mathbf{e}_2') + a_2(\mathbf{e}_1\mathbf{e}_3' - \mathbf{e}_3\mathbf{e}_1') + a_1(\mathbf{e}_3\mathbf{e}_2' - \mathbf{e}_2\mathbf{e}_3')$$

with $\mathbf{e}_j$ being the jth unit vector of size 3×1. From this it follows that

$$\mathbf{T_a} = \sum_{j=1}^{3} a_j \mathbf{T}_{\mathbf{e}_j}.$$

The vector cross product can also be calculated by determinants:

$$\mathbf{a} \times \mathbf{b} = \left(\det \begin{pmatrix} a_2 & b_2 \\ a_3 & b_3 \end{pmatrix},\ \det \begin{pmatrix} a_3 & b_3 \\ a_1 & b_1 \end{pmatrix},\ \det \begin{pmatrix} a_1 & b_1 \\ a_2 & b_2 \end{pmatrix} \right)'.$$

As the product is used in Physics and in Engineering, we now list some further properties.

Theorem 11. *For* $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, $\mathbf{d}$ *of size* 3×1 *and scalars* α *and* β, *we have*

$$
\begin{aligned}
&(54) & \mathbf{T}_{\alpha\mathbf{a}+\beta\mathbf{b}} &= \alpha\mathbf{T}_{\mathbf{a}} + \beta\mathbf{T}_{\mathbf{b}}, \\
&(55) & \mathbf{T}_{\mathbf{a}}\mathbf{b} &= -\mathbf{T}_{\mathbf{b}}\mathbf{a}, \\
&(56) & \mathbf{T}_{\mathbf{a}} &= -\mathbf{T}'_{\mathbf{a}}, \\
&(57) & \mathbf{T}_{\mathbf{a}}\mathbf{a} &= \mathbf{0}, \\
&(58) & \mathbf{T}_{\mathbf{a}}\mathbf{T}_{\mathbf{b}} &= \mathbf{b}\mathbf{a}' - \mathbf{a}'\mathbf{b}\mathbf{I}_3, \\
&(59) & (\mathbf{T}_{\mathbf{a}}\mathbf{T}_{\mathbf{b}})' &= \mathbf{T}_{\mathbf{b}}\mathbf{T}_{\mathbf{a}}, \\
&(60) & \mathbf{T}_{\mathbf{a}}\mathbf{T}_{\mathbf{b}}\mathbf{T}_{\mathbf{c}} &= \mathbf{T}_{\mathbf{a}}\mathbf{c}\mathbf{b}' - \mathbf{b}'\mathbf{c}\mathbf{T}_{\mathbf{a}}, \\
&(61) & \mathbf{T}_{\mathbf{a}}\mathbf{T}_{\mathbf{b}}\mathbf{T}_{\mathbf{a}} &= -\mathbf{a}'\mathbf{b}\mathbf{T}_{\mathbf{a}}, \\
&(62) & \mathbf{T}_{\mathbf{a}}\mathbf{T}_{\mathbf{a}}\mathbf{T}_{\mathbf{a}} &= -\mathbf{a}'\mathbf{a}\mathbf{T}_{\mathbf{a}}, \\
&(63) & \mathbf{c}'\mathbf{T}_{\mathbf{a}}\mathbf{b} &= \mathbf{a}'\mathbf{T}_{\mathbf{b}}\mathbf{c} = \mathbf{b}'\mathbf{T}_{\mathbf{c}}\mathbf{a} = -\mathbf{c}'\mathbf{T}_{\mathbf{b}}\mathbf{a} = -\mathbf{b}'\mathbf{T}_{\mathbf{a}}\mathbf{c} = -\mathbf{a}'\mathbf{T}_{\mathbf{c}}\mathbf{b}, \\
&(64) & \mathbf{T}_{\mathbf{a}}\mathbf{T}_{\mathbf{b}}\mathbf{c} &= (\mathbf{a}'\mathbf{c})\mathbf{b} - (\mathbf{a}'\mathbf{b})\mathbf{c} = \mathbf{a} \times (\mathbf{b} \times \mathbf{c}), \ \textit{Grassmann's Identity} \\
& & (\mathbf{T}_{\mathbf{a}}\mathbf{b})'(\mathbf{T}_{\mathbf{c}}\mathbf{d}) &= (\mathbf{a}'\mathbf{c})(\mathbf{b}'\mathbf{d}) - (\mathbf{a}'\mathbf{d})(\mathbf{b}'\mathbf{c}), \ \textit{Lagrange's Identity} \\
&(65) & &= (\mathbf{a} \times \mathbf{b})'(\mathbf{c} \times \mathbf{d}), \\
&(66) & \mathbf{T}_{\mathbf{T}_{\mathbf{a}}\mathbf{b}} &= \mathbf{b}\mathbf{a}' - \mathbf{a}\mathbf{b}' = \mathbf{T}_{\mathbf{a}}\mathbf{T}_{\mathbf{b}} - \mathbf{T}_{\mathbf{b}}\mathbf{T}_{\mathbf{a}}, \\
&(67) & \mathbf{T}_{\mathbf{a}}{}^{+} &= -\frac{1}{\mathbf{a}'\mathbf{a}}\mathbf{T}_{\mathbf{a}}, \ \text{if } \mathbf{a} \neq \mathbf{0}.
\end{aligned}
$$

Note that $\mathbf{c}'\mathbf{T}_{\mathbf{a}}\mathbf{b}$ is just the scalar triple product $(\mathbf{abc}) = (\mathbf{a} \times \mathbf{b})'\mathbf{c}$. For these and more results, see Trenkler (1998, 2001, 2002), Gross et al. (1999, 2001), Neudecker et al. (2003) and Neudecker and Trenkler (2005, 2006a). For further properties, we refer to Bernstein (2005, Fact 3.5.25).

3.8. Results involving Khatri-Rao sum. The following is a new result.

Theorem 12. *For compatibly partitioned* $\mathbf{A}$, $\mathbf{A}^{-1}$, $\mathbf{B}$ *and* $\mathbf{B}^{-1}$ *with eigenvalues contained in the interval* $[\lambda, \mu]$, *we have*

$$
(68) \qquad 4\mathbf{I} \leq \mathbf{A} \diamond \mathbf{B}^{-1} + \mathbf{A}^{-1} \diamond \mathbf{B} \leq \frac{2(\lambda + \mu)}{\lambda^{1/2}\mu^{1/2}}\,\mathbf{I}.
$$

A special case is when the Khatri-Rao product becomes the Hadamard product where the block sub-matrices are actually the elements themselves. This special case generalizes Corollaries 4.1 and 4.2, both by Al Zhour and Kilicman (2006b).

4. Applications

The results involving the Hadamard product are in fact two examples of applications of the Hadamard product. Below we focus on the Khatri-Rao product.

4.1. Variances in Statistics and Econometrics. Sims et al. (1990) considered estimation and hypothesis testing in linear time series regressions with unit roots. Chambers et al. (1998) discussed limited information maximum likelihood estimation for analysis of survey data. They derived respectively two variance matrices each containing a Khatri-Rao product. We can find sufficient (and necessary) conditions for the two covariance matrices to be strictly positive definite.

The first covariance matrix can written as

$$
\boldsymbol{\Psi} = \boldsymbol{\Omega} * \mathbf{W},
$$

where

$$\begin{aligned} \mathbf{\Omega} &= \begin{pmatrix} \mathbf{\Sigma} & \mathbf{\Sigma} \\ \mathbf{\Sigma} & \mathbf{\Sigma} \end{pmatrix} \geq \mathbf{0}, \quad \mathbf{\Sigma} \geq \mathbf{0}, \\ \mathbf{W} &= \begin{pmatrix} \mathbf{\Gamma}_1\mathbf{\Gamma}_1' & \mathbf{\Gamma}_1\mathbf{\Gamma}_2' \\ \mathbf{\Gamma}_2\mathbf{\Gamma}_1' & \mathbf{\Gamma}_2\mathbf{\Gamma}_2' \end{pmatrix} \geq \mathbf{0}, \quad \mathbf{\Gamma_1\Gamma_1'} > \mathbf{0}. \end{aligned}$$

For the definitions of the relevant submatrices above and detail background, see Sims et al. (1990) and Banerjee et al. (1993). Obviously, (33) in Theorem 6 ensures in an algebraic approach that $\mathbf{\Psi} \geq \mathbf{0}$, as $\mathbf{\Omega} \geq \mathbf{0}$ and $\mathbf{W} \geq \mathbf{0}$. In practice, an important question is to examine when $\mathbf{\Psi} > \mathbf{0}$ is positive definite. By using (36) in Theorem 6 we get the answer: $\mathbf{\Psi} > \mathbf{0}$ is equivalent to $\mathbf{\Sigma} > \mathbf{0}$ with $\mathbf{W} > \mathbf{0}$, i.e. $\mathbf{\Sigma} > \mathbf{0}$ with $\mathbf{\Gamma}_2\mathbf{\Gamma}_2' - \mathbf{\Gamma}_2\mathbf{\Gamma}_1'(\mathbf{\Gamma}_1\mathbf{\Gamma}_1')^{-1}\mathbf{\Gamma}_1\mathbf{\Gamma}_2' > \mathbf{0}$, as $\mathbf{\Gamma}_1\mathbf{\Gamma}_1' > \mathbf{0}$ is assumed.

The second covariance matrix is

$$\mathbf{\Lambda} = \mathbf{P} * \mathbf{Q},$$

where

$$\mathbf{P} = \begin{pmatrix} \mathbf{R} & \mathbf{R} \\ \mathbf{R} & \mathbf{I}_n \end{pmatrix} \geq \mathbf{0}, \quad \mathbf{Q} = \begin{pmatrix} h & \mathbf{c}' \\ \mathbf{c} & \mathbf{\Sigma} \end{pmatrix},$$

$\mathbf{R} = \mathbf{I}_n - \frac{1}{N}\mathbf{1}_n\mathbf{1}_n' > \mathbf{0}$, $N > n+1$, $h > 0$ is a scalar, $\mathbf{\Sigma} > \mathbf{0}$ is a $(q+1) \times (q+1)$ variance matrix, and $\mathbf{c}$ is a $(q+1) \times 1$ vector.

Also, Chambers et al. (1998) used $t_1 = h - \mathbf{c}'\mathbf{\Sigma}^{-1}\mathbf{c}$ (which is a scalar), and gave necessary details. We are interested in when $\mathbf{\Lambda} > \mathbf{0}$. Based on (35) in Theorem 6, we specify $\mathbf{\Lambda} > \mathbf{0}$ if $t_1 > 0$ which is equivalent to $\mathbf{Q} > \mathbf{0}$ as $\mathbf{\Sigma} > \mathbf{0}$ ($\mathbf{\Lambda} \geq \mathbf{0}, \mathbf{\Lambda} \not> \mathbf{0}$, if $t_1 = 0$). Such a (sufficient) condition is useful and efficient because it is quite easy to check.

4.2. Multi-way models and algorithms. In multivariate statistics, psychometrics, engineering, food and chemical sciences, among other areas, multi-way data, models and algorithms have received significant attention for about a decade. The Khatri-Rao product plays an important role.

We start with a two-way bilinear or PCA (principal component analysis) model: given data matrix $\mathbf{X}$ and the (same) column-dimension of loading matrices $\mathbf{A}$ and $\mathbf{B}$, fit the model $\hat{\mathbf{X}} = \mathbf{AB}'$ as the solution to minimize $\mathrm{tr}(\mathbf{X} - \mathbf{AB}')'(\mathbf{X} - \mathbf{AB}')$ subject to $\mathbf{A}'\mathbf{A} = \mathbf{D}$ and $\mathbf{B}'\mathbf{B} = \mathbf{I}$, where $\mathbf{D}$ is a diagonal matrix and $\mathbf{I}$ is an identity matrix. As shown by Bro (1998, ch. 3), this model can be extended to one of the three-way PARAFAC (PARAllel FACtor) models which is represented by using the Khatri-Rao product in the column-wise partitioned case as follows

$$\mathbf{X} = \mathbf{A}(\mathbf{C} * \mathbf{B})' + \mathbf{E},$$

where $\mathbf{X}$ is the three-way data matrix, $\mathbf{C}*\mathbf{B}$ replaces $\mathbf{B}$ to reflect the same (parallel) profiles only in different proportions for the model, and $\mathbf{E}$ is the approximation error matrix. Here it is evident that the Khatri-Rao product makes model specification easy and transparent, especially for high-order PARAFAC models. For example, a four-way PARAFAC model can simply be written as

$$\mathbf{X} = \mathbf{A}(\mathbf{F} * \mathbf{C} * \mathbf{B})' + \mathbf{E},$$

where $\mathbf{F}$ is the fourth mode loading matrix. Several extensions and variations of the PARAFAC model and other models including PARAFAC2, PARATUCK2 and

N-PLS (a general multi-way partial least squares regression) can be represented using the Khatri-Rao product.

The Khatri-Rao product is also useful in the algorithms for estimating the parameters. As an example, consider now the (error-free) three-way PARAFAC model

$$\mathbf{X} = \mathbf{A}(\mathbf{C} * \mathbf{B})'.$$

To estimate $\mathbf{A}, \mathbf{B}$ and $\mathbf{C}$, an alternating least squares algorithm can be used (otherwise to estimate the parameters *simultaneously* using least squares is a rather difficult nonlinear problem); see Bro (1998, pp. 57-65). To illustrate how powerful the Khatri-Rao product is, we just take one step of the loop for the algorithm. That is: we initialize $\mathbf{B}$ and $\mathbf{C}$ for $\mathbf{X} = \mathbf{A}\mathbf{Z}'$, i.e. (69); we then find the conditional estimate $\mathbf{A} = \mathbf{X}\mathbf{Z}(\mathbf{Z}'\mathbf{Z})^{+}$; see Box 5 given by Bro (1998, p. 63). Here we point out that $\mathbf{Z}'\mathbf{Z} = \mathbf{C}'\mathbf{C} \odot \mathbf{B}'\mathbf{B}$ can be obtained by using (25) and its Moore-Penrose inverse $(\mathbf{Z}'\mathbf{Z})^{+} = (\mathbf{C}'\mathbf{C} \odot \mathbf{B}'\mathbf{B})^{+}$ by (26). The same idea applies to higher-order models. Consider e.g. a four-way model with $\mathbf{Z} = \mathbf{F} * \mathbf{C} * \mathbf{B}$. Then $\mathbf{Z}'\mathbf{Z} = \mathbf{F}'\mathbf{F} \odot \mathbf{C}'\mathbf{C} \odot \mathbf{B}'\mathbf{B}$ using (25). Clearly such expressions for $\mathbf{Z}'\mathbf{Z}$ and its Moore-Penrose inverse involving the Khatri-Rao product *indeed* allow efficient computations. Bro (1998, p. 65) notes that the calculations can be done efficiently, though if implemented in MATLAB (1998 or earlier), such expressions would need to be compiled or rewritten in a vectorial way to function efficiently. Bro (1998, p. 64) also presents a nice result for using an existing PARAFAC model on new data. In such a situation, we are interested in estimating the scores of one or several new samples. With $\mathbf{B}$ and $\mathbf{C}$ given from the prior obtained model, the solution to the problem is simply a least squares problem and can be easily given by using (27). We refer to Bro (1998) for details of these algorithms and other issues and results with applications.

For further detailed and more results on multi-way data, PARAFAC models, algorithms, validation and constraints, and on other associated models, data analysis and applications in psychometrics, signal processing, chemometrics and food sciences, see e.g. Bro (1998), Ten Berge and Sidiropoulos (2002), Jiang and Sidiropoulos (2004), Smilde et al. (2004) and Tomasi and Bro (2006).

4.3. Linear matrix equations. Linear matrix equations show up in a variety of mathematics, physics and engineering problems, including linear system analysis, modelling of non-stationary covariances and multi-static antenna array processing. For example, the generalized Lyapunov equation

$$\mathbf{A}\mathbf{X}\mathbf{B}' + \mathbf{C}\mathbf{X}\mathbf{D}' = \mathbf{Q}$$

has been used to characterize structured covariance matrices, and to construct efficient matrix factorization and inversion algorithms; see e.g. Lev-Ari (2005). The following equation is studied by Lev-Ari (2005) which is of somewhat different flavour taken in multi-static antenna array processing applications. An unknown medium is probed by transmitting energy into it from a multi-element antenna array, and recording the scattered signal received by (another) multi-element antenna array. The resulting measurements are arranged into a matrix

$$\mathbf{H} = \mathbf{G}_{\mathrm{rec}}\mathbf{X}\mathbf{G}_{\mathrm{tr}}', \tag{69}$$

where the $l \times l$ multi-static data matrix $\mathbf{H} = (h_{ij})$, h_{ij} is the response (at a single frequency) from the jth transmitting element to the ith receiving element, the $l \times l$ unknown matrix $\mathbf{X} = \mathrm{diag}(\tau_i)$ is diagonal with τ_i as scattering coefficients,

$\mathbf{G}_{\text{rec}} = (g_{\text{rec}}(\chi_1), \ldots, g_{\text{rec}}(\chi_l))$, $\mathbf{G}_{\text{tr}} = (g_{\text{tr}}(\chi_1), \ldots, g_{\text{tr}}(\chi_l))$, χ_i indicates the scatter locations, $g_{\text{tr}}(\chi_i)$ (resp. $g_{\text{rec}}(\chi_1)$) is the steering vector associated with wave propagation between the transmitting (resp. receiving) array and the ith scatterer, $i, j = 1, \ldots, l$, where l is the number of point scatterers. We now have to find our solution to linear matrix equation (69) with respect to $\mathbf{X}$. First we use (27) to get

$$\begin{aligned} \operatorname{vec}(\mathbf{H}) &= (\mathbf{G}_{\text{tr}} \otimes \mathbf{G}_{\text{rec}}) \operatorname{vec}(\mathbf{X}) \\ &= (\mathbf{G}_{\text{tr}} \otimes \mathbf{G}_{\text{rec}}) \mathbf{J} \operatorname{vecd}(\mathbf{X}) \\ &= (\mathbf{G}_{\text{tr}} * \mathbf{G}_{\text{rec}}) \operatorname{vecd}(\mathbf{X}) \end{aligned}$$

and then use (25) and (26) to get

$$\begin{aligned} \operatorname{vecd}(\mathbf{X}) &= [(\mathbf{G}_{\text{tr}} * \mathbf{G}_{\text{rec}})'(\mathbf{G}_{\text{tr}} * \mathbf{G}_{\text{rec}})]^{-1} (\mathbf{G}_{\text{tr}} * \mathbf{G}_{\text{rec}})' \operatorname{vec}(\mathbf{H}) \\ &= [(\mathbf{G}_{\text{tr}}'\mathbf{G}_{\text{tr}}) \odot (\mathbf{G}_{\text{rec}}'\mathbf{G}_{\text{rec}})]^{-1} (\mathbf{G}_{\text{tr}} * \mathbf{G}_{\text{rec}})' \operatorname{vec}(\mathbf{H}) \\ &= [(\mathbf{G}_{\text{tr}}'\mathbf{G}_{\text{tr}}) \odot (\mathbf{G}_{\text{rec}}'\mathbf{G}_{\text{rec}})]^{-1} \operatorname{vecd}(\mathbf{G}_{\text{rec}}'\mathbf{H}\mathbf{G}_{\text{tr}}). \end{aligned} \tag{70}$$

As pointed by Lev-Ari (2005), the above solution is much more efficient than the one using the following well-known formula:

$$\operatorname{vec}(\mathbf{X}) = [(\mathbf{G}_{\text{tr}} \otimes \mathbf{G}_{\text{rec}})'(\mathbf{G}_{\text{tr}} \otimes \mathbf{G}_{\text{rec}})]^{-1} (\mathbf{G}_{\text{tr}} \otimes \mathbf{G}_{\text{rec}})' \operatorname{vec}(\mathbf{H}),$$

as most of the elements of $\mathbf{X}$ in this solution are useless except for the diagonal elements which only are needed. Note that $(\mathbf{G}_{\text{tr}}'\mathbf{G}_{\text{tr}}) \odot (\mathbf{G}_{\text{rec}}'\mathbf{G}_{\text{rec}})$ in (70) is invertible as both $\mathbf{G}_{\text{rec}}$ and $\mathbf{G}_{\text{tr}}$ have full column rank, except in very rare pathological cases where we have to use the Moore-Penrose inverse instead.

4.4. Signal processing. Space-time coding techniques exploit the spatial diversity afforded by multiple transmitting and receiving antennas to achieve reliable transmission in scattering-rich environments. Sidiropoulos and Budampati (2002) propose a broad new class of space-time codes based on the Khatri-Rao product, KRST codes, for short. They report that KRST codes are linear block codes designed to provide several benefits, which yield better performance than linear dispersion codes at high signal-to-noise ratio and than linear constellation precoding codes using a lower order constellation. Consider the multi-antenna system with M transmitting antennas and N receiving antennas. The wireless channel is assumed to be quasi-static and flat fading. The discrete-time baseband-equivalent model for the received data is given (when the channel is constant for at least K channel uses) by

$$\mathbf{X} = \sqrt{\frac{\rho}{M}}\mathbf{H}\mathbf{C} + \mathbf{W},$$

where $\mathbf{X}$ is the $N \times K$ received signal matrix, $\mathbf{C}$ is the $M \times K$ transmitted code matrix, $\mathbf{W}$ is the $N \times K$ additive noise matrix, $\mathbf{H}$ is the $N \times M$ channel matrix which has i.i.d. $N(0, 1)$ entries being mutually independent from $\mathbf{X}$ and $\mathbf{W}$, and ρ is the signal-to-noise ratio. In Sidiropoulos and Budampati's (2002) discussion, the resulting transmitted code matrix is given by $\mathbf{C}_t = \mathbf{D}(\boldsymbol{\Theta}\mathbf{s}_t)\mathbf{C}_0'$ (with the construction of $\mathbf{C}_0'$ addressed) for the situation under study, and if the channel is assumed to be constant for block time T the received data can be modelled as

$$\begin{aligned} \mathbf{X}_t &= \sqrt{\frac{\rho}{M}}\mathbf{H}\mathbf{C}_{\mathbf{t}} + \mathbf{W}_{\mathbf{t}} \\ &= \sqrt{\frac{\rho}{M}}\mathbf{H}\mathbf{D}(\boldsymbol{\Theta}\mathbf{s}_t)\mathbf{C}_0' + \mathbf{W}_t, \ t = 1, \ldots, T. \end{aligned} \tag{71}$$

For further specifications of the model and preliminaries, see e.g. Sidiropoulos and Budampati (2002). Using the Khatri-Rao product and (27), for the channel assumed to be constant for block time T we obtain the following (noiseless) vectorized model

$$\begin{aligned}\operatorname{vec}\mathbf{X}_t &= \sqrt{\frac{\rho}{M}}(\mathbf{C}_0 * \mathbf{H})\operatorname{vecd}(\mathbf{D}(\boldsymbol{\Theta}\mathbf{s}_t)) \\ &= \sqrt{\frac{\rho}{M}}(\mathbf{C}_0 * \mathbf{H})\boldsymbol{\Theta}\mathbf{s}_t. \qquad (72)\end{aligned}$$

Then using (26) the transmitted symbol vector $\mathbf{s}_t$ can be recovered by

$$\begin{aligned}\mathbf{s}_t &= (\sqrt{\frac{\rho}{M}}(\mathbf{C}_0 * \mathbf{H})\boldsymbol{\Theta})^{+}\operatorname{vec}\mathbf{X}_t \\ &= [\sqrt{\frac{\rho}{M}}\boldsymbol{\Theta}'(\mathbf{C}_0 * \mathbf{H})'(\mathbf{C}_0 * \mathbf{H})\boldsymbol{\Theta}]^{+}\boldsymbol{\Theta}'(\mathbf{C}_0 * \mathbf{H})'\operatorname{vec}\mathbf{X}_t \\ &= [\sqrt{\frac{\rho}{M}}\boldsymbol{\Theta}'(\mathbf{C}_0'\mathbf{C}_0 \odot \mathbf{H}'\mathbf{H})\boldsymbol{\Theta}]^{+}\boldsymbol{\Theta}'(\mathbf{C}_0 * \mathbf{H})'\operatorname{vec}\mathbf{X}_t, \qquad (73)\end{aligned}$$

for almost every $\mathbf{H}$ with the particular choice of $\mathbf{C}_0$, as $\boldsymbol{\Theta}$ is a unitary $M \times M$ matrix.

Based on the Khatri-Rao product, Wang et al. (2006) consider a similar data model and propose a novel Khatri-Rao unitary space-time modulation design. Their idea is to use the Khatri-Rao product to obtain a decomposition result to find a simplified maximum likelihood detection algorithm for their design. Upon the decomposition the new detector needs to perform only a *vector* multiplication, instead of a *matrix* multiplication which the original detector needs to perform. As reported the new design does not require any computer search and can be applied to any number of transmitting antennas, among other improvements.

Note that Sidiropoulos and Budampati (2002) have also made PARAFAC analysis involving the Khatri-Rao product. For further studies on the Khatri-Rao product used in signal processing problems, see also e.g. Yu and Petropulu (2006) and others.

5. Concluding remarks

We have collected several basic results on the Hadamard, Khatri-Rao, Tracy-Singh, Kronecker and vector cross products, and with the Khatri-Rao and Tracy-Singh sums each as a variation of the Khatri-Rao and Tracy-Singh products, respectively. As our attempt to draw attention to the matrix products, we have also presented four examples involving particularly the Khatri-Rao product and its applications in not only statistics, econometrics and psychometrics, but also physics, engineering, chemometrics and food sciences. However, we note that the majority of applications of the Khatri-Rao product is still based on only the column-wise partitioned situation. Note also that the Khatri-Rao and Tracy-Singh products cannot be dealt with directly say by built-in functions in the commonly used computer languages or packages so far, although the Kronecker and vector cross products can be (MATLAB has a command `kron` for calculating the Kronecker product of two matrices, and MAPLE has `CrossProduct` and MATHEMATICA has `Cross` both for the vector cross product of two three-dimensional vectors; see e.g. Hogben, 2006, pp. 71-4, 72-3 and 73-5). It is hoped to have a wider range of applications of the

Khatri-Rao (in the matrix-wise partitioned case) and other products with a number of supportive computer built-in functions or packages before long.

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