

# KRONECKER SQUARE ROOTS AND THE BLOCK VEC MATRIX

IGNACIO OJEDA

ABSTRACT. Using the block vec matrix, I give a necessary and sufficient condition for factorization of a matrix into the Kronecker product of two other matrices. As a consequence, I obtain an elementary algorithmic procedure to decide whether a matrix has a square root for the Kronecker product.

## INTRODUCTION

My statistician colleague, J.E. Chacón, asked me how to decide if a real given matrix  $A$  has a square root for the Kronecker product (i.e., if there exists a  $B$  such that  $A = B \otimes B$ ) and, in the positive case, how to compute it. His questions were motivated by the fact that, provided that a certain real positive definite symmetric matrix has a Kronecker square root, explicit asymptotic expressions for certain estimator errors could be obtained. See [1], for a discussion of the importance of multivariate kernel density derivative estimation.

This note is written mostly due to the lack of a suitable reference for the existence of square roots for the Kronecker product, and it is organized as follows: first of all, I study the problem of the factorization of a matrix into a Kronecker product of two matrices, by giving a necessary and sufficient condition under which this happens (Theorem 3). As a preparation for the main result, I introduce the *block vec matrix* (Definition 1). Now, the block vec matrix and Theorem 3 solve our problem in a constructive way.

### 1. KRONECKER PRODUCT FACTORIZATION

Throughout this note  $\mathbb{N}$ ,  $\mathbb{R}$ , and  $\mathbb{C}$  denote the sets of non-negative integers, real numbers, and complex numbers, respectively. All matrices considered here have real or complex entries;  $A^\top$  denotes the transpose of  $A$  and  $\text{tr}(A)$  denotes its trace.

The operator that transforms a matrix into a stacked vector is known as the *vec operator* (see, [3, Definition 4.2.9] or [6, § 7.5]). If  $A = (\mathbf{a}_1 | \dots | \mathbf{a}_n)$  is an  $m \times n$  matrix whose columns are  $\mathbf{a}_1, \dots, \mathbf{a}_n$ , then  $\text{vec}(A)$  is the  $mn \times 1$  matrix

$$\text{vec}(A) = \begin{pmatrix} \mathbf{a}_1 \\ \vdots \\ \mathbf{a}_n \end{pmatrix}.$$

The following definition generalizes the vec operation and is the key to all that follows.

**Definition 1.** Let  $A = (A_{ij})$  be an  $mp \times nq$  matrix partitioned into block matrices  $A_{ij}$ , each of order  $p \times q$ . The block vec matrix of  $A$  corresponding to the given partition is the  $mn \times pq$  matrix

$$\text{vec}^{(p \times q)}(A) = \begin{pmatrix} A_1 \\ \vdots \\ A_n \end{pmatrix}, \quad \text{where each } A_j = \begin{pmatrix} \text{vec}(A_{1j})^\top \\ \vdots \\ \text{vec}(A_{mj})^\top \end{pmatrix}.$$

If  $A$  is  $m \times n$ , it is instructive to verify the following identities corresponding to four natural ways to partition it:

- $p = q = 1$  :  $\text{vec}^{(1 \times 1)}(A) = \text{vec}(A)$ ,
- $p = m, q = n$  :  $\text{vec}^{(m \times n)}(A) = \text{vec}(A)^\top$ ,
- $p = 1, q = n$  (partition by rows):  $\text{vec}^{(1 \times n)}(A) = A$ ,
- $p = m, q = 1$  (partition by columns):  $\text{vec}^{(m \times 1)}(A) = A^\top$ .

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If  $A$  is  $mp \times nq$  and  $\text{vec}(A)$  is partitioned into  $nq$  blocks, each of size  $mp \times 1$ , then a computation reveals that  $\text{vec}^{(mp \times 1)}(\text{vec}(A)) = A^\top$ .

Let  $B = (b_{ij})$  be an  $m \times n$  matrix and let  $C$  be a  $p \times q$  matrix. The *Kronecker product* of  $B$  and  $C$ , denoted by  $B \otimes C$ , is the  $mp \times nq$  matrix

$$B \otimes C = \begin{pmatrix} b_{11}C & b_{12}C & \cdots & b_{1n}C \\ b_{21}C & b_{22}C & \cdots & b_{2n}C \\ \vdots & \vdots & & \vdots \\ b_{m1}C & b_{m2}C & \cdots & b_{mn}C \end{pmatrix}.$$

The following result is straightforward; see [7, Theorem 1].

**Lemma 2.** *Let  $B$  be an  $m \times n$  matrix and let  $C$  be a  $p \times q$  matrix. Then*

$$\text{vec}^{(p \times q)}(B \otimes C) = \text{vec}(B)\text{vec}(C)^\top.$$

*In particular,  $\text{vec}^{(p \times q)}(B \otimes C)^\top = \text{vec}^{(m \times n)}(C \otimes B)$ .*

It may be (but need not) be possible to factor a given matrix, suitably partitioned, as a Kronecker product of two other matrices. For example, a zero matrix can always be factored as a Kronecker product of a zero matrix and any matrix of suitable size. The following theorem provides a necessary and sufficient condition for a Kronecker factorization.

**Theorem 3.** *Let  $A = (A_{ij})$  be a nonzero  $mp \times nq$  matrix, partitioned into blocks of order  $p \times q$ . There exist matrices  $B$  (of order  $m \times n$ ) and  $C$  (of order  $p \times q$ ) such that  $A = B \otimes C$  if and only if  $\text{rank}(\text{vec}^{(p \times q)}(A)) = 1$ .*

*Proof.* If  $A = B \otimes C$  is a factorization of the stated form, then  $B, C, \text{vec}(B)$ , and  $\text{vec}(C)$  must all be nonzero. Lemma 2 ensures that

$$\text{rank}(\text{vec}^{(p \times q)}(A)) = \text{rank}(\text{vec}^{(p \times q)}(B \otimes C)) = \text{rank}(\text{vec}(B)\text{vec}(C)^\top) = 1.$$

Conversely, since  $A \neq 0$ , there are indices  $r$  and  $s$  such that  $A_{rs} \neq 0$  and hence  $\text{vec}(A_{rs}) \neq 0$ . Since  $\text{rank}(\text{vec}^{(p \times q)}(A)) = 1$ , each row of  $\text{vec}^{(p \times q)}(A)$  is a scalar multiple of any nonzero row. Thus, there are scalars  $b_{ij}$  such that each  $\text{vec}(A_{ij}) = b_{ij} \text{vec}(A_{rs})$ . This means that  $A = B \otimes C$ , in which  $B = (b_{ij})$  and  $C = A_{rs}$ .  $\square$

Notice that the preceding proof provides a simple construction for a pair of Kronecker factors for  $A$  if  $\text{rank}(\text{vec}^{(p \times q)}(A)) = 1$ .

The block  $\text{vec}$  matrix can be used to detect not only whether a given matrix has a Kronecker factorization of a given form, but also, if it does not, how closely it can be approximated in the Frobenius norm by a Kronecker product. A best approximation is determined by the singular value decomposition of the block  $\text{vec}$  matrix. For details, see [7], where the block  $\text{vec}$  matrix is called the *rearrangement matrix*.

*Example 4.* Consider

$$A = \begin{pmatrix} 2 & 1 \\ 2 & 0 \\ 3 & 0 \\ 0 & 3 \end{pmatrix}.$$

Since

$$\text{vec}^{(2 \times 2)}(A) = \begin{pmatrix} 2 & 2 & 1 & 0 \\ 3 & 0 & 0 & 3 \end{pmatrix}$$

has rank 2, Theorem 3 ensures that  $A \neq B \otimes C$ , for any  $B$  and  $C$  of order  $2 \times 1$  and  $2 \times 2$ , respectively.

The set of matrices that factorizes into the Kronecker product of two other matrices have the following interpretation in Algebraic Geometry.

*Remark 5.* Let  $A$  be a real  $mp \times nq$  matrix and consider the big matrix

$$M = \begin{pmatrix} I_{mn} \otimes \mathbf{u}_{pq}^\top \\ \mathbf{u}_{mn}^\top \otimes I_{pq} \end{pmatrix}$$

where  $\mathbf{u}_\bullet$  is the all-ones vector of dimension  $\bullet$ . Let  $K$  be equal to  $\mathbb{R}$  or  $\mathbb{C}$  and let

$$\varphi_M : K[X_{11}, \dots, X_{m1}, X_{12}, \dots, X_{mn}, X_{pq}] \longrightarrow K[t_1, \dots, t_{mn+pq}]$$

be the  $K$ -algebra map such that  $\varphi(\mathbf{X}^{\mathbf{u}}) = \mathbf{t}^{M\mathbf{u}}$ , with  $\mathbf{X}^{\mathbf{u}} := X_{11}^{u_1} \cdots X_{mn\ pq}^{u_{mn+pq}}$  and  $\mathbf{t}^{\mathbf{v}} := t_1^{v_1} \cdots t_{mn+pq}^{v_{mn+pq}}$ . Then  $X = (x_{ij})$  has rank 1 if and only if  $\text{vec}(X)^\top$  is a zero of  $\ker \varphi_M$  (see, e.g. [2, Section 2]). Therefore, by Theorem 3, the set of  $mn \times pq$  matrices which factor into the Kronecker product of an  $m \times n$  matrix and a  $p \times q$  matrix is the following *algebraic set*

$$\mathcal{V}(\ker \varphi_M) = \left\{ A \in K^{mn \times pq} \mid \text{vec}(\text{vec}^{(p \times q)}(A))^\top \in \ker \varphi_M \right\}.$$

In Algebraic Statistics,  $\ker \varphi_M$  is the ideal associated to two independent random variables with values in  $\{1, \dots, mn\}$  and  $\{1, \dots, pq\}$ . Thus, as it is well known in Statistics, *factorization means independence and vice versa*.

We can now give a solution to the problem that motivates this paper.

**Corollary 6.** *If  $A$  is a nonzero  $m^2 \times n^2$  matrix and  $B$  an  $n \times n$  matrix, then*

- (a)  $A = B \otimes B$  if and only if  $\text{vec}^{(m \times n)}(A) = \text{vec}(B)\text{vec}(B)^\top$ ,
- (b) if  $A = B \otimes B$ , then  $\text{vec}^{(m \times n)}(A)$  is symmetric and has rank one.

Is the necessary condition in the preceding corollary sufficient? It is not surprising that the answer depends on the field. For example, if  $m = n = 1$  and  $A = (-1)$ , then  $\text{vec}^{(1 \times 1)}(A) = (-1)$  is symmetric and has rank one, but  $A$  has no real Kronecker square root; it does have complex Kronecker square roots  $B = (\pm i)$ , but these are the only ones.

**Theorem 7.** *Let  $A$  be an  $m^2 \times n^2$  real or complex matrix. Suppose that  $\text{vec}^{(m \times n)}(A)$  is symmetric and has rank one.*

- (a) *There is an  $m \times n$  matrix  $B$  such that  $A = B \otimes B$ .*
- (b) *If  $B$  and  $C$  are  $m \times n$  matrices such that  $A = B \otimes B = C \otimes C$ , then  $C = \pm B$ .*
- (c) *If  $A$  is real, there is a real  $m \times n$  matrix  $B$  such that  $A = B \otimes B$  if and only if  $\text{tr}(\text{vec}^{(m \times n)}(A)) > 0$ .*

*Proof.* Any complex symmetric matrix has a special singular value decomposition, that is unique in a certain way; see [4, Corollary 4.4.4: Autonne's theorem]. In the case of a rank one symmetric matrix  $Z$  whose largest (indeed, only nonzero) singular value is  $\sigma$ , Autonne's theorem says that there is a unit vector  $\mathbf{u}$  such that  $Z = \sigma \mathbf{u} \mathbf{u}^\top$ . Moreover, if  $\mathbf{v}$  is a unit vector such that  $Z = \sigma \mathbf{v} \mathbf{v}^\top$ , then  $\mathbf{v} = \pm \mathbf{u}$ . If we use Autonne's theorem to represent the block vec matrix as  $\text{vec}^{(m \times n)}(A) = \sigma \mathbf{u} \mathbf{u}^\top = (\sigma^{1/2} \mathbf{u})(\sigma^{1/2} \mathbf{u})^\top$  and define  $B$  by  $\text{vec}(B) = (\sigma^{1/2} \mathbf{u})$ , we have  $\text{vec}^{(m \times n)}(A) = \text{vec}(B)\text{vec}(B)^\top$ . The preceding corollary now ensures that  $A = B \otimes B$  and the assertion in (b) follows from the uniqueness part of Autonne's theorem.

Now suppose that  $A$  is real. If there is a real  $B$  such that  $A = B \otimes B$ , then  $\text{tr}(\text{vec}^{(m \times n)}(A)) = \text{tr}(\text{vec}(B)\text{vec}(B)^\top) = \text{vec}(B)^\top B$  is positive since it is the square of the Euclidean norm of the (necessarily nonzero) real vector  $\text{vec}(B)$ . Conversely, the spectral theorem ensures that any real symmetric matrix can be represented as  $Q\Lambda Q^\top$ , in which  $Q$  is real orthogonal and  $\Lambda$  is real diagonal. Since the block vec matrix is real symmetric and has rank one, we can take  $\Lambda = \text{diag}(\lambda, 0, \dots, 0)$  and represent  $\text{vec}^{(m \times n)}(A) = \lambda \mathbf{q} \mathbf{q}^\top$  in which  $\mathbf{q}$  is the first column of  $Q$ . If  $\lambda = \text{tr}(\text{vec}^{(m \times n)}(A)) > 0$ , then  $\text{vec}^{(m \times n)}(A) = (\lambda^{1/2} \mathbf{q})(\lambda^{1/2} \mathbf{q})^\top = \text{vec}(B)\text{vec}(B)^\top$ , in which  $\text{vec}(B) = \lambda^{1/2} \mathbf{q}$  (and hence also  $B$ ) is real.  $\square$

The uniqueness part of the preceding theorem has some perhaps surprising consequences.

**Corollary 8.** *Let  $A$  be a nonzero  $m^2 \times n^2$  real or complex matrix and suppose that  $A = B \otimes B$  for some  $m \times n$  matrix  $B$ .*

- (a)  *$A$  is symmetric if and only if  $B$  is either symmetric or skew symmetric.*
- (b)  *$A$  is not skew symmetric.*
- (c)  *$A$  is Hermitian if and only if  $B$  is either Hermitian or skew Hermitian.*
- (d)  *$A$  is Hermitian positive definite if and only if  $B$  is Hermitian and definite (positive or negative).*
- (e)  *$A$  is skew Hermitian if and only if  $e^{i\pi/4} B$  is Hermitian.*
- (f)  *$A$  is unitary if and only if  $B$  is unitary.*
- (g) *If  $B$  is real, then  $A$  is real orthogonal if and only if  $B$  is real orthogonal.*
- (h)  *$A$  is complex orthogonal if and only if either  $B$  or  $iB$  is complex orthogonal.*

*Proof.* (a)  $A^\top = B^\top \otimes B^\top$ , so  $A = A^\top$  if and only if  $A = B \otimes B = B^\top \otimes B^\top$ , which holds if and only if  $B^\top = \pm B$ .

(b) If  $A^\top = -A^\top$ , then  $-A = -B \otimes B = (iB) \otimes (iB) = B^\top \otimes B^\top$  and hence  $B^\top = \pm iB = \pm i(B^\top)^\top = \pm i(\pm iB)^\top = -B^\top$ , so  $B = 0$ .

(c)  $A = A^*$  if and only if  $A = B \otimes B = B^* \otimes B^*$ , that is to say,  $B^* = \pm B$ .

(d) Using (c) and the fact that the eigenvalues of  $B \otimes B$  are the pairwise products of the eigenvalues of  $B$ , we can exclude the possibility that  $B$  is skew Hermitian since in that case its nonzero eigenvalues (there must be at least one) would be pure imaginary and hence  $B \otimes B$  would have at least one negative eigenvalue.

(e) Under our hypothesis, the following statements are equivalent (i)  $A = -A^*$ , (ii)  $A = B \otimes B = -B^* \otimes B^* = (iB)^* \otimes (iB)^*$  (iii)  $B^* = \pm iB$  (iv)  $(e^{i\pi/4}B)^* = \pm e^{i\pi/4}B$ , and so the claim follows.

(f)  $A^{-1} = B^{-1} \otimes B^{-1} = B^* \otimes B^*$  if and only if  $B^* = \pm B^{-1}$  or, that is the same,  $BB^* = \pm I$ . However  $BB^* = -I$  is not possible since  $BB^*$  is positive definite.

(g) Follows from (f).

(h)  $A^{-1} = B^{-1} \otimes B^{-1} = B^\top \otimes B^\top$  if and only if  $B^\top = \pm B^{-1}$  that is to say  $BB^\top = \pm I$  or, equivalently, either  $BB^\top = I$  or  $(iB)(iB)^\top = I$ .  $\square$

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DEPARTAMENTO DE MATEMÁTICAS, UNIVERSIDAD DE EXTREMADURA, E-06071 BADAJOZ, ESPAÑA.  
E-mail address: ojedadmc@unex.es