Products of positive semi-definite matrices

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Dedicated to Professor Rajendra Bhatia.

Abstract

It is known that every complex square matrix with nonnegative determinant is the product of positive semi-definite matrices. There are characterizations of matrices that require two or five positive semi-definite matrices in the product. However, the characterizations of matrices that require three or four positive semi-definite matrices in the product are lacking. In this paper, we give a complete characterization of these two types of matrices. With these results, we give an algorithm to determine whether a square matrix can be expressed as the product of $k$ positive semi-definite matrices but not fewer, for $k = 1, 2, 3, 4, 5$.

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1 Introduction

Let $M_n$ be the set of $n \times n$ complex matrices. In [3], the author showed that a matrix in $M_n$ with nonnegative determinant can always be written as the product of five or fewer positive semi-definite matrices. This is an extension to the result in [1] asserting that every matrix in $M_n$ with positive determinant is the product of five or fewer positive definite matrices. Analogous to the analysis in [1], the author of [3] studied those matrices which can be expressed as the product of two, three, or four positive semi-definite matrices. In particular, characterization was obtained for the matrices that can be expressed as the product of two semi-definite matrices; also, it was shown that any matrices not of the form $zI$, where $z$ is not a nonnegative number, could be written as the product of four positive semi-definite matrices. Moreover, it was proved in [3, Theorem 3.3] that if one applies a unitary similarity to change the square matrix to the form $T = \begin{bmatrix} T_1 & * \\ 0 & T_2 \end{bmatrix} \in M_n$ such that $T_1$ is invertible and $T_2$ is nilpotent, and if $T_1$ is the product of three positive definite matrices, then $T$ can be expressed as the product of three positive semi-definite matrices as well. It was suspected that the converse of this statement is also true. However, the following example shows that it is not the case.

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Example 1.1 Let $T = \begin{bmatrix} -9 & -9 \\ 0 & 0 \end{bmatrix}$. Then $T = \begin{bmatrix} 9 & 3 \\ 3 & 2 \end{bmatrix} \begin{bmatrix} 13 & -15 \\ -15 & 18 \end{bmatrix} \begin{bmatrix} 1 & 1 \end{bmatrix}$ is the product of three positive semi-definite matrices. However, $T_1 = [-9]$ is not the product of three positive definite matrices because $\det(T_1) < 0$.

Of course, one may impose the obvious necessary condition that $\det(T_1) > 0$, and ask whether the conjecture is valid with this additional assumption. Nevertheless, it is easy to modify Example 1 by considering $T \otimes I_2 = \begin{bmatrix} -9I_2 \\ 0 \end{bmatrix} = (A_1 \otimes I_2)(A_2 \otimes I_2)(A_3 \otimes I_3)$ using the factorization $T = A_1A_2A_3$. In the modified example, we have $T_1 = -9I_2$ and $T_2 = 0_2$. By [1, Theorem 4], $T_1 = -9I_2$ is the product of no fewer than five positive definite matrices.

In the next section, we will give a complete characterization for those matrices that can be written as the product of three positive semi-definite matrices and not fewer. Also, we add an easy to check necessary and sufficient condition for invertible matrices that can be written as the product of three positive definite matrices. With these results, one can use the Jordan form of a given matrix and its numerical range to decide whether it can be expressed as the product of two, three, four or five positive semi-definite matrices.

2 Product of three positive semi-definite matrices

We will prove the following.

Theorem 2.1 Suppose 

$$T = \begin{bmatrix} T_1 & R \\ 0 & T_2 \end{bmatrix} \text{ such that } T_1 \text{ is invertible and } T_2 \text{ is nilpotent. }$$

(1) Then $T$ is a product of three positive semi-definite matrices if and only if one of the following holds.

(a) $R \neq 0$ or $T_2 \neq 0$.

(b) $R = 0$, $T_2 = 0$, and $T_1$ is the product of three positive definite matrices.

We establish some lemmas to prove Theorem 2.1. The first one is covered by [1, Theorem 1].

Lemma 2.2 Let $A, S \in M_n$ such that $S$ is invertible. Then $A$ is a product of an odd number of positive semi-definite matrices if and only if $S^*AS$ is.

In the next lemma, we need the concept of the numerical range of a matrix $A \in M_n$ defined by

$$W(A) = \{ x^*Ax : x \in \mathbb{C}^n, x^*x = 1 \}.$$ 

The numerical range is a useful tool in studying matrices. One may see [2, Chapter 1] for the basic properties of the numerical range.
Lemma 2.3 Suppose \( T = \begin{bmatrix} T_1 & R \\ 0 & 0_p \end{bmatrix} \) such that \( T_1 \in M_m \) is invertible and \( R \) is nonzero. Then \( T \) is a product of three positive semi-definite matrices.

Proof. First, we show that there is a \( p \times m \) matrix \( S \) such that \( T_1 + RS \) is the product of three positive definite matrices.

If \( m = 1 \), there is \( S \in \mathbb{C}^p \) such that \( T_1 + RS > 0 \). Suppose \( m > 1 \) and \( R \) has a singular value decomposition \( R = s_1 x_1 y_1^* + \cdots + s_k x_k y_k^* \), where \( s_1, \ldots, s_k \) are nonzero singular values of \( R \), and \( x_1, \ldots, x_k \in \mathbb{C}^m \) and \( y_1, \ldots, y_k \in \mathbb{C}^p \) are their corresponding right and left unit singular vectors accordingly. Let \( \{ e_1, \ldots, e_m \} \) be the standard basis for \( \mathbb{C}^m \). Take a unitary \( U \) such that \( Ux_1 = e_1 \). Since \( T_1 \) is invertible, so is \( \hat{T}_1 = UT_1 U^* \). Suppose \( \hat{t}_1 \) is the first row of \( \hat{T}_1 \). Let \( v = \hat{t}_1 + e_2 \) with \( \epsilon > 0 \) and \( \hat{T}_1(\epsilon) \) be the \( m \times m \) matrix obtained from \( \hat{T}_1 \) by replacing its first row with \( v^* \). Take a sufficiently small \( \epsilon > 0 \) such that \( v \) is not a multiple of \( e_1 \) and the matrix \( \hat{T}_1(\epsilon) \) is still invertible.

Set \( S = s_1^{-1} e^{i\theta} y_1 v^* U \) with \( r > 0 \) and \( \theta \in [0, 2\pi) \). Then

\[
U(T_1 + RS)U^* = UT_1 U^* + URSU^* = \hat{T}_1 + re^{i\theta} e_1 v^*.
\]

Since \( v \) is not a multiple of \( e_1 \), the rank one matrix \( e_1 v^* \) is not normal and so \( W(e_1 v^*) \) is an elliptical disk with foci 0 and \( v_1 \) with length of minor axis \( \sqrt{\|v^*\|^2 - |v_1|^2} > 0 \), where \( v_1 \) is the first entry of \( v \); for example, see [2] Theorem 1.3.6. By the fact that the map \( X \mapsto W(X) \) is continuous, for a sufficiently large \( r > 0 \), \( W(e_1 v^* + e^{-i\theta} \hat{T}_1/r) \) still contains 0 as an interior point for any \( \theta \in [0, 2\pi) \). Then so does

\[
W(\hat{T}_1 + re^{i\theta} e_1 v^*) = re^{i\theta} W(e_1 v^* + \frac{e^{-i\theta}}{r} \hat{T}_1).
\]

In addition, the value \( r \) can be chosen so that \( r > |\det(\hat{T}_1)/\det(\hat{T}_1(\epsilon))| \). Now by the linearity of determinant with respect to the first row,

\[
\det(T_1 + RS) = \det(U(T_1 + RS)U^*) = \det(\hat{T}_1 + re^{i\theta} e_1 v^*) = \det(\hat{T}_1) + re^{i\theta} \det(\hat{T}_1(\epsilon)).
\]

Since \( |\det(\hat{T}_1)| < |re^{i\theta} \det(\hat{T}_1(\epsilon))| \), there is \( \theta \in [0, 2\pi) \) such that \( \det(T_1 + RS) > 0 \). By [1] Theorem 3 (see also Proposition 2.4), \( T_1 + RS \) is a product of three positive definite matrices.

Finally, note that

\[
\hat{T} = \begin{bmatrix} I_m & S^* \\ 0 & I_p \end{bmatrix} \begin{bmatrix} T_1 & R \\ 0 & 0_p \end{bmatrix} \begin{bmatrix} I_m & 0 \\ S & I_p \end{bmatrix} = \begin{bmatrix} T_1 + RS & R \\ 0 & 0_p \end{bmatrix}.
\]

By [3] Theorem 3.3, \( \hat{T} \) is a product of three positive semi-definite matrices, and so is \( T \) by Lemma 2.2. \( \square \)

Proof of Theorem 2.1 Suppose \( T \) is the product of three positive semi-definite matrices. If \( R \neq 0 \) or \( T_2 \neq 0 \), then we are done. Else, \( T = T_1 \oplus 0_p \) is the product of three positive semi-definite matrices. By [3] Proposition 3.5, \( T_1 \) is the product of three positive definite matrices.
To prove the converse, we consider the following three cases.

**Case 1.** Suppose $R \neq 0$. We use induction on $p$, the size of $T_2$. If $p = 1$, the result follows from Lemma 2.3 as $T_2 = [0]$. Assume the result holds for $T_2$ with size at most $p-1$. Since $T_2$ is nilpotent, without loss of generality, we may assume that $T_2$ is upper triangular with $T_2 = \begin{bmatrix} T_{21} & T_{22} \\ 0 & 0 \end{bmatrix}$, where $T_{21} \in M_{p-1}$. Write $R = \begin{bmatrix} R_1 & R_2 \end{bmatrix}$ where $R_1$ is $m \times (p-1)$. If $R_1 \neq 0$, then by induction, the matrix $\begin{bmatrix} T_{11} & R_1 \\ 0 & T_{21} \end{bmatrix}$ is a product of three positive semi-definite matrices, say, $P_1P_2P_3$. Further, by [3, Theorem 2.2] (see also Proposition 3.1), we may assume that both $P_1$ and $P_2$ are invertible. Let $X = \begin{bmatrix} R_2 \\ T_{22} \end{bmatrix}$ with size $(m + p - 1) \times 1$. Then for any $\epsilon > 0$,

$$
\begin{bmatrix}
P_1 \\ 0
\end{bmatrix} \begin{bmatrix}
P_2 \\ 0
\end{bmatrix} \begin{bmatrix}
\epsilon P_1^{-1}X \\ 1
\end{bmatrix} \begin{bmatrix}
P_3 \\ 0
\end{bmatrix} = \begin{bmatrix}
P_1P_2P_3X \\ 0
\end{bmatrix} = \begin{bmatrix}
T_{11} & R_1 & R_2 \\ 0 & T_{21} & T_{22}
\end{bmatrix} = T.
$$

Clearly, $Q_1 = P_1 \oplus [0]$ and $Q_3 = P_3 \oplus [\epsilon^{-1}]$ are positive semi-definite matrices. Now one can choose a sufficiently small $\epsilon > 0$ so that $Q_2 = \begin{bmatrix}
P_2 \\ \epsilon(P_1^{-1}X)^* \\ 1
\end{bmatrix}$ is also positive semi-definite. Thus, $T$ is a product of three positive semi-definite matrices $Q_1Q_2Q_3$.

Now suppose $R_1 = 0$. Then the $(m+1)$th column of $T$ is a zero column. By interchanging the $(m+1)$th and the last indices, one can see that $T$ is permutationally similar to

$$
\begin{bmatrix}
T_{11} & \tilde{R} & 0 \\ 0 & \tilde{T}_{21} & 0 \\ 0 & \tilde{T}_{22} & 0
\end{bmatrix}
$$

where $\tilde{R}$ is $m \times (p-1)$, $\tilde{T}_{21}$ is $(p-1) \times (p-1)$, and $\tilde{T}_{22}$ is $1 \times (p-1)$.

Notice also that $\tilde{R}$ is nonzero and $\tilde{T}_{21}$ is nilpotent. By induction, $\begin{bmatrix}
T_{11} & \tilde{R} \\ 0 & \tilde{T}_{21}
\end{bmatrix}$ is a product of three positive semi-definite matrices $P_1P_2P_3$. By [3, Theorem 2.2], we can further assume that both $P_2$ and $P_3$ are invertible. Let $Y = \begin{bmatrix}
0 & \tilde{T}_{22}
\end{bmatrix}$ with size $1 \times (m + p - 1)$. Then for any $\epsilon > 0$,

$$
\begin{bmatrix}
P_1 \\ 0
\end{bmatrix} \begin{bmatrix}
P_2 \\ 0
\end{bmatrix} \begin{bmatrix}
\epsilon(Y P_3^{-1})^* \\ 1
\end{bmatrix} \begin{bmatrix}
P_3 \\ 0
\end{bmatrix} = \begin{bmatrix}
P_1P_2P_3Y \\ 0
\end{bmatrix} = \begin{bmatrix}
T_{11} & \tilde{R} & 0 \\ 0 & \tilde{T}_{21} & \tilde{T}_{22}
\end{bmatrix}.
$$

Again, one can choose a sufficiently small $\epsilon > 0$ such that all three matrices in the left side of the above equation are positive semi-definite. Thus, $T$ is permutationally similar to a product of three positive semi-definite matrices, and hence $T$ can also be written as a product of three positive semi-definite matrices.

**Case 2.** Suppose $R = 0$ and $T_2$ is nonzero. Without loss of generality, we may assume that $T_2$ is upper triangular with zero diagonal entries while the first row of $T_2$ is nonzero. Let $Z$ be the
$p \times m$ matrix with 1 at the (1,1)-entry and zero elsewise. Then $Z^*T_2 \neq 0$ and $T_2Z = 0$. Let $S = \begin{bmatrix} I_m & 0 \\ Z & I_p \end{bmatrix}$. Then

$$S^*TS = \begin{bmatrix} I_m & Z^* \\ 0 & I_p \end{bmatrix} \begin{bmatrix} T_1 & 0 \\ 0 & T_2 \end{bmatrix} \begin{bmatrix} I_m & 0 \\ Z & I_p \end{bmatrix} = \begin{bmatrix} T_1 + Z^*T_2Z & Z^*T_2 \\ T_2Z & T_2 \end{bmatrix} = \begin{bmatrix} T_1 & Z^*T_2 \\ 0 & T_2 \end{bmatrix}.$$ 

Since $Z^*T_2 \neq 0$, the result follows from Case 1 and Lemma 2.2.

**Case 3.** Suppose $R = 0$ and $T_2 = 0$. If $T_1$ is the product of three positive definite matrices, then $T = T_1 \oplus 0_p$ is the product of three positive semi-definite matrices. \hfill \Box

Note that Theorem 2.1 depends on checking an invertible matrix is the product of three positive definite matrices. Such conditions are given in [1, Theorem 3]. We restated the result in terms of the numerical range in the following proposition, which is based on the discussion in [1, Theorem 3 and Fact 3.2].

**Proposition 2.4** Let $T \in M_n$ be such that $\det(T) > 0$. Then $T$ is the product of three positive definite matrices if and only if one of the following holds.

(a) $W(T)$ contains 0 as an interior point.

(b) $W(T)$ contains a positive number, and the arguments of the eigenvalues of $T$ can be arranged as: $-\pi < \theta_1 \leq \cdots \leq \theta_n < \pi$ such that $\sum_{j=1}^{n} \theta_j = 0$.

Note that in [1, p.88], the author required in condition (3.6b), corresponding to our condition (b), that all real eigenvalues of $T$ are positive, which is ensured by our assumption that $\theta_j \in (-\pi, \pi)$ for all $j$.

### 3 Determining the number of factors

In this section, we describe an algorithm to determine the smallest number of positive semi-definite matrices whose product equals a given $A \in M_n$ with nonnegative determinant.

We first present the following theorem providing some easy tests for a matrix $A$ to be the product of two positive semi-definite matrices. The equivalence of conditions (a), (b), (c) were given in [3, Theorem 2.2]. We include a short proof, which is different from that of Wu.

**Proposition 3.1** Let $A$ be a square matrix. The following are equivalent.

(a) $A$ is the product of two positive semi-definite matrices.

(b) $A = BC$, where $B, C$ are positive semi-definite matrices such that $B$ or $C$ can be assumed to be invertible.

(c) $A$ is similar to a nonnegative diagonal matrix.
(d) A is unitarily similar to an upper block triangular matrix such that the diagonal blocks are scalar matrices corresponding to distinct scalars.

(c) The minimal polynomial of $A$ only has simple nonnegative zeros.

Proof. The equivalence of (c), (d), (e) are clear.

(c) $\Rightarrow$ (b): $A = S^{-1}DS = S^{-1}(S^{-1})^*(S^*DS) = S^{-1}D(S^{-1})^*(S^*S)$.

(b) $\Rightarrow$ (a): Trivial.

(a) $\Rightarrow$ (c): Suppose $A = BC$, where $B$ and $C$ are $n \times n$ positive semi-definite. Let $U$ be unitary such that $U^*BU = B_0 \oplus 0_k$, where $B_0 \in M_{n-k}$ is positive definite. Let $U^*CU = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}$ be such that $C_{22} \in M_k$. Assume $V$ is unitary such that $V^*C_{11}V = C_0 \oplus 0_\ell$ for a positive definite matrix $C_0 \in M_{n-k-\ell}$. We may replace $U$ by $U(V \oplus I)$ and assume that $C_{11} = C_0 \oplus 0_\ell$. Because $C$ is positive semi-definite, $U^*CU = \begin{bmatrix} C_0 & 0 & C_1 \\ 0 & 0_\ell & 0 \\ C_{1*} & 0 & C_{22} \end{bmatrix}$. Then

$$U^*AU = \begin{bmatrix} B_0 & 0 \\ 0 & 0_k \end{bmatrix} \begin{bmatrix} C_0 & 0 & C_1 \\ 0 & 0_\ell & 0 \\ C_{1*} & 0 & C_{22} \end{bmatrix} = \begin{bmatrix} B_0 & 0 \\ 0 & 0_\ell \end{bmatrix} \begin{bmatrix} C_0 & 0 & C_1 \\ 0 & 0_\ell & 0 \\ 0 & 0 & 0_k \end{bmatrix}.$$ 

Now

$$\begin{bmatrix} B_0^{-\frac{1}{2}} & 0 \\ 0 & I_k \end{bmatrix} \begin{bmatrix} I & 0 & C_0^{-1}C_1 \\ 0 & I & 0 \\ 0 & 0 & I_k \end{bmatrix} \begin{bmatrix} B_0 & 0 \\ 0 & 0_k \end{bmatrix} \begin{bmatrix} C_0 & 0 & C_1 \\ 0 & 0_\ell & 0 \\ 0 & 0 & 0_k \end{bmatrix} \begin{bmatrix} B_0^\frac{1}{2} & 0 \\ 0 & I_k \end{bmatrix}$$

$$= \begin{bmatrix} B_0^{-\frac{1}{2}} & 0 \\ 0 & I_k \end{bmatrix} \begin{bmatrix} B_0 & 0 \\ 0 & 0_k \end{bmatrix} \begin{bmatrix} C_0 & 0 & 0 \\ 0 & 0_\ell & 0 \\ 0 & 0 & 0_k \end{bmatrix} \begin{bmatrix} B_0^\frac{1}{2} \\ 0 \end{bmatrix} = \begin{bmatrix} B_0^\frac{1}{2} \\ 0 \end{bmatrix} = \begin{bmatrix} B_0^\frac{1}{2} \end{bmatrix} \begin{bmatrix} C_0 & 0 \\ 0 & 0_\ell \end{bmatrix} \begin{bmatrix} B_0^\frac{1}{2} \\ 0 \end{bmatrix} \oplus 0_k.$$

Therefore, $A$ is similar to $\begin{bmatrix} B_0^\frac{1}{2} & 0 \\ 0 & 0_\ell \end{bmatrix} \begin{bmatrix} C_0 & 0 \\ 0 & 0_\ell \end{bmatrix} \begin{bmatrix} B_0^\frac{1}{2} \\ 0 \end{bmatrix} \oplus 0_k$, which is positive semi-definite and is (unitarily) similar to a nonnegative diagonal matrix.

Now, we are ready to present an algorithm to check whether a matrix $A \in M_n$ with $\det(A) \geq 0$ can be written as a product of $k$ positive semi-definite matrices, but not fewer, for $k = 1, 2, 3, 4, 5$.

**Algorithm 3.2** Let $A \in M_n$ with $\det(A) \geq 0$.

If $A = \alpha I_n$ such that $\alpha \notin [0, \infty)$, then $A$ can be expressed as a product of five positive semi-definite matrices, but not fewer. Otherwise, apply a unitary similarity to $A$ to get an upper triangular matrix $T = \begin{bmatrix} T_1 & R \\ 0 & T_2 \end{bmatrix}$ such that $T_1$ is invertible and $T_2$ is nilpotent.
If $T$ is a nonnegative diagonal matrix, then $A$ is itself a positive semi-definite matrix.

(2) Condition (1) does not hold, and $A$ satisfies any one of the equivalent conditions in Proposition 3.1. Then $A$ can be expressed as a product of two positive semi-definite matrices, but not fewer.

(3) Suppose (1) and (2) do not hold. Then $A$ can be expressed as a product of three positive semi-definite matrices, but not fewer, if any of the following holds.

(3.a) $R$ or $T_2$ is nonzero.

(3.b) Both $R = 0$ and $T_2 = 0$, and $T_1$ is the product of three positive definite matrices.

In (3.b), the invertible matrix $T_1$ is a product of three positive definite matrices if one of the following holds.

(i) $\det(T_1) > 0$ and $W(T_1)$ contains 0 as an interior point,

(ii) 0 is not in the interior of $W(T_1)$ and $W(T_1)$ contains a positive number and $\sum \theta_j = 0$, where $-\pi < \theta_1 \leq \cdots \leq \theta_k < \pi$ are the arguments of the eigenvalues of $T_1$.

(4) Suppose conditions (1), (2), (3) do not hold, i.e., $T = T_1 \oplus 0_p$ such that neither (i) nor (ii) holds for the upper triangular matrix $T_1$. Then $A$ can be expressed as a product of four positive semi-definite matrices, but not fewer.

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