A characterization theorem for matrix variances

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Abstract

Some recent papers formulated sufficient conditions for the decomposition of matrix variances [6, 10]. A statement was that if we have one or two observables, then the decomposition is possible. In this paper we consider an arbitrary finite set of observables and we present a necessary and sufficient condition for the decomposition of the matrix variances.

The subject here is matrix theory, see [1, 4, 7]. By a density matrix $D \in M_n(\mathbb{C})$ we mean $D \geq 0$ and $\text{Tr} D = 1$. In quantum information theory the traditional variance is defined by

$$\text{Var}_D(A) = \text{Tr} DA^2 - (\text{Tr} DA)^2,$$

where $D$ is a density matrix and $A \in M_n(\mathbb{C})$ is a self-adjoint operator. This noncommutative variance is a natural extension of the variance in probability theory [2], and has several applications [3, 4, 5, 8, 9, 10]. It is easy to show that

$$\text{Var}_D(A + \lambda I) = \text{Var}_D(A) \quad (\lambda \in \mathbb{R})$$

and the concavity of the variance functional is well-known:

$$\text{Var}_D(A) \geq \sum_i \lambda_i \text{Var}_{D_i}(A),$$

when $D = \sum_i \lambda_i D_i$, $\lambda_i \geq 0$ and $\sum_i \lambda_i = 1$. It was proved in [10] that for every self-adjoint operator $A$ and density matrix $D$ there are projections $P_k$ such that $D = \sum_k \lambda_k P_k$ with $0 < \lambda_k$, $\sum_k \lambda_k = 1$ and $\text{Var}_D(A) = \sum_k \lambda_k \text{Var}_{P_k}(A)$ holds.

There is another example when the previous $A$ is replaced with $A_1, A_2, \ldots, A_r$, they are also self-adjoint operators. Then the standard variance is a matrix in $M_r(\mathbb{C})$:

$$[\text{Var}_D(A_1, \ldots, A_r)]_{i,j} = \text{Tr} DA_i A_j - (\text{Tr} DA_i)(\text{Tr} DA_j) \quad (1 \leq i, j \leq r).$$

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Assume that $0 \leq \lambda_1, \lambda_2$ and $\lambda_1 + \lambda_2 = 1$. An elementary computation gives that

$$\left[ \text{Var}_{\lambda_1 D_1 + \lambda_2 D_2}(A_1, \ldots, A_r) - \lambda_1 \text{Var}_{D_1}(A_1, \ldots, A_r) - \lambda_2 \text{Var}_{D_2}(A_1, \ldots, A_r) \right]_{ij} = \lambda_1 \lambda_2 a_i a_j,$$

where

$$a_i = \text{Tr} (D_1 - D_2) A_i, \quad 1 \leq i \leq r.$$

It follows that

$$\text{Var}_{\lambda_1 D_1 + \lambda_2 D_2}(A_1, \ldots, A_r) \geq \lambda_1 \text{Var}_{D_1}(A_1, \ldots, A_r) + \lambda_2 \text{Var}_{D_2}(A_1, \ldots, A_r).$$

So we have the concavity of the variance functional $D \mapsto \text{Var}_D(A_1, \ldots, A_r)$:

$$\text{Var}_D(A_1, \ldots, A_r) \geq \sum_i \lambda_i \text{Var}_{D_i}(A_1, \ldots, A_r) \quad \text{if} \quad D = \sum_i \lambda_i D_i,$$

where $\lambda_i \geq 0$ and $\sum_i \lambda_i = 1$. For $r = 2$ the equality may be also true and this is the result in [6]: $D$ is a certain convex combination of projections $P_k$ as $D = \sum_k p_k P_k$ and

$$\text{Var}_D(A_1, A_2) = \sum_k p_k \text{Var}_{P_k}(A_1, A_2).$$

In the present paper we give a necessary and sufficient condition for the previous equality for an arbitrary set $\{A_1, \ldots, A_r\}$ of self-adjoint operators.

1 General computations

As it was declared, the variance functional is concave, that is, if $D_1, \ldots, D_m$ are density matrices, $A_1, \ldots, A_r$ are self-adjoint operators and $D = \sum_{k=1}^m \lambda_k D_k$ with some $0 \leq \lambda_1, \ldots, \lambda_m$, $\sum_{k=1}^m \lambda_k = 1$ then

$$\text{Var}_D(A_1, \ldots, A_r) \geq \sum_{k=1}^m \lambda_k \text{Var}_{D_k}(A_1, \ldots, A_r). \quad (1)$$

We are interested in the case of equality in (1).

**Lemma.** If $D_1, \ldots, D_m$ are density matrices, $A_1, \ldots, A_r$ are self-adjoint operators and $D = \sum_{k=1}^m \lambda_k D_k$ with some $0 < \lambda_1, \ldots, \lambda_m$, $\sum_{k=1}^m \lambda_k = 1$, then

$$\text{Var}_D(A_1, \ldots, A_r) = \sum_{k=1}^m \lambda_k \text{Var}_{D_k}(A_1, \ldots, A_r) \quad (2)$$

if and only if

$$\text{Tr}_{D_k} A_j = \text{Tr} D A_j \quad \text{for all} \quad 1 \leq k \leq m \quad \text{and} \quad 1 \leq j \leq r. \quad (3)$$
Proof: The variance has the shift invariance property

\[ \text{Var}_D(A_1, \ldots, A_r) = \text{Var}_D(A_1 - \lambda_1 I, \ldots, A_r - \lambda_r I) \]

for every reals \( \lambda_1, \ldots, \lambda_r \). Set \( \lambda_j := \text{Tr}DA_j \). With this choice \( \text{Tr}D(A_j - \lambda_j I) = 0 \) holds for every \( j \). Therefore

\[ [\text{Var}_D(A_1, \ldots, A_r)]_{ij} = [\text{Var}_D(A_1 - \lambda_1 I, \ldots, A_r - \lambda_r I)]_{ij} = \text{Tr}D(A_i - \lambda_i I)(A_j - \lambda_j I). \]

Because of the concavity of the variance,

\[ \text{Var}_D(A_1, \ldots, A_r) - \sum_{k=1}^{m} \lambda_k \text{Var}_{D_k}(A_1, \ldots, A_r) \]

is a positive semi-definite matrix, hence it is equal to zero if and only if the diagonal elements are zeros, that is,

\[ \text{Tr}D(A_j - \lambda_j I)^2 - \left( \sum_{k=1}^{m} \lambda_k \text{Tr}D_k(A_j - \lambda_j I)^2 - \lambda_k (\text{Tr}D_k(A_j - \lambda_j I))^2 \right) = 0 \quad (4) \]

holds for every \( j \). It is easy to check that (4) holds if and only if \( \text{Tr}D_k(A_j - \lambda_j I) = 0 \) for every \( k, j \) and this is equivalent to (3).

\[ \square \]

In the next section we use this Lemma to characterize those sets of self-adjoint operators for which the decomposition of the matrix variances with projections is possible.

2 The main theorem

Let us introduce some notations:

\[ M_n^{sa}(\mathbb{C}) := \{ A \in M_n(\mathbb{C}) : A^* = A \}, \]

\[ M_n^+(\mathbb{C}) := \{ C \in M_n(\mathbb{C}) : C \geq 0 \}, \]

\[ S(\mathbb{C}^n) := \{ D \in M_n(\mathbb{C}) : D \geq 0, \text{Tr}D = 1 \}. \]

For an arbitrary subspace \( \mathcal{K} \subset \mathbb{C}^n \), we denote by \( Q^K \) the orthogonal projection onto \( \mathcal{K} \). We define

\[ A^K := Q^K A Q^K \]

for every operator \( A \in M_n(\mathbb{C}) \) and

\[ B(\mathcal{K}) := Q^K M_n(\mathbb{C}) Q^K, \quad B^{sa}(\mathcal{K}) := Q^K M_n^{sa}(\mathbb{C}) Q^K, \]

\[ B^+(\mathcal{K}) := Q^K M_n^+(\mathbb{C}) Q^K, \quad S(\mathcal{K}) := \{ X \in B^+(\mathcal{K}) : \text{Tr}X = 1 \}. \]
**Definition.** Let \( \{A_1, \ldots, A_r\} \) be a set of self-adjoint operators in \( M_n(\mathbb{C}) \). \( \{A_1, \ldots, A_r\} \) is said to be variance-decomposable if for every \( D \in \mathcal{S}(\mathbb{C}^n) \) there exist \( P_1, \ldots, P_m \) rank-one projections such that

\[
D = \sum_{k=1}^{m} \lambda_k P_k \quad \text{and} \quad \text{Var}_D(A_1, \ldots, A_r) = \sum_{k=1}^{m} \lambda_k \text{Var}_{P_k}(A_1, \ldots, A_r)
\]

with some \( 0 \leq \lambda_k \), \( \sum_k \lambda_k = 1 \).

**Theorem.** \( \{A_1, \ldots, A_r\} \subset M_n(\mathbb{C}) \) is variance-decomposable if and only if

\[
\dim \left( \text{span} \{ I^K, A^K_1, \ldots, A^K_r \} \right) < (\dim K)^2
\]

for every \( K \subset \mathbb{C}^n \) subspace with \( \dim K > 1 \).

Note that this theorem immediately shows that every set of self-adjoint operators with at most two elements is variance-decomposable. (This is the result of [10] and [6].)

**Proof:** By the Lemma, \( \{A_1, \ldots, A_r\} \subset M_n(\mathbb{C}) \) is variance-decomposable if and only if for every \( D \in \mathcal{S}(\mathbb{C}^n) \) density operator there exist \( P_1, \ldots, P_m \) rank-one projections such that

\[
D \in \text{Conv} \{ P_1, \ldots, P_m \} \quad \text{-- where Conv}(H) \text{ denotes the convex hull of the set } H --
\]

and

\[
\text{Tr} P_k A_j = \text{Tr} D A_j \quad \text{for all } 1 \leq k \leq m \text{ and } 1 \leq j \leq r.
\]

We show that the condition (5) is sufficient. It is enough to show that for every \( D \in \mathcal{S}(\mathbb{C}^n) \), \( \text{rank}(D) > 1 \) there exist \( E_1, \ldots, E_m \in \mathcal{S}(\mathbb{C}^n) \) density operators such that

\[
D \in \text{Conv} \{ E_1, \ldots, E_m \}
\]

and

\[
\text{Tr} E_k A_j = \text{Tr} D A_j \quad \text{for all } k \text{ and } j
\]

and

\[
\text{rank}(E_k) < \text{rank}(D).
\]

Let \( D \) be an arbitrary element of \( \mathcal{S}(\mathbb{C}^n) \) with \( \text{rank}(D) > 1 \), \( K := \text{range}(D) \). \( B^{sa}(K) \) is a \( (\dim(K))^2 \) dimensional Hilbert space over the field \( \mathbb{R} \) with the positive definite inner product \( \langle X, Y \rangle = \text{Tr} XY \). Let us use the notation \( A = (A_1, \ldots, A_r) \). Define

\[
\mathcal{L}^K_{D,A} := \{ X \in B^{sa}(K) : \langle X, I \rangle = 1, \langle X, A_j \rangle = \langle D, A_j \rangle \quad \text{for all } j \}.
\]

Clearly,

\[
\mathcal{L}^K_{D,A} = \{ X \in B^{sa}(K) : \langle X, I^K \rangle = 1, \langle X, A^K_j \rangle = \langle D, A^K_j \rangle \quad \text{for all } j \}.
\]

Because of the assumption \( \dim \left( \text{span} \{ I^K, A^K_1, \ldots, A^K_r \} \right) < (\dim K)^2 \), \( \mathcal{L}^K_{D,A} \) is an affine subspace of \( B^{sa}(K) \) with positive dimension.
It is well-known that \( S(K) \) is a bounded convex set (for example, \( \|P\|_2 \leq 1 \) if \( P \in S(K) \), where \( \|\cdot\|_2 \) denotes the Hilbert-Schmidt norm). Therefore, \( L^K_{D,A} \cap S(K) \) is a bounded convex set and
\[
L^K_{D,A} \cap S(K) \subset \text{Conv} \left( L^K_{D,A} \cap \partial S(K) \right),
\]
where \( \partial S(K) \) denotes the relative boundary of \( S(K) \).

By definition, \( D \in L^K_{D,A} \cap S(K) \), and hence
\[
D = \sum_{k=1}^m \lambda_k E_k \quad \text{with some } \{E_k\}_{k=1}^m \subset L^K_{D,A} \cap \partial S(K) \quad \text{and } 0 \leq \lambda_k, \sum \lambda_k = 1.
\]
This is exactly the statement we wanted to prove, because \( E_k \in \partial S(K) \) implies that \( \text{rank}(E_k) < \dim(K) = \text{rank}(D) \), that is, (9) holds, and \( E_k \in L^K_{D,A} \) implies that (8) holds.

Note that \( D \) has a maximal rank in \( S(K) \), hence it is a (relative) interior point of \( S(K) \). On the other hand, \( L^K_{D,A} \) lies in the affine hull of \( S(K) \) and has a positive dimension. Therefore, the intersection \( L^K_{D,A} \cap S(K) \) is not a single point.

To show that the condition (5) is necessary as well, assume that
\[
\dim \left( \text{span} \{ I^K, A^K_1, \ldots, A^K_r \} \right) = (\dim K)^2
\]
for some \( K \subset \mathbb{C}^n \) subspace with \( \dim K > 1 \). Set \( D \in S(K) \), \( \text{rank}(D) > 1 \). Because of the assumption \( \dim \left( \text{span} \{ I^K, A^K_1, \ldots, A^K_r \} \right) = (\dim K)^2 \), \( L^K_{D,A} \) is a 0 dimensional affine subspace of \( B^{sa}(K) \), that is, \( L^K_{D,A} = \{D\} \). Therefore, we have by Lemma that the decomposition of \( D \) is impossible. \( \square \)

The next example shows that for an arbitrary large \( n \) there exists a set of self-adjoint operators with only three elements which is not variance-decomposable.

**Example.** For every \( n \geq 2 \) we can show \( A_1, A_2, A_3 \in M_n(\mathbb{C}) \) self-adjoint matrices and a \( D \in S(\mathbb{C}^n) \) density with the following property. If \( P_1, \ldots, P_m \) are rank-one projections such that \( D = \sum_{k=1}^m \lambda_k P_k \) with some \( 0 < \lambda_1, \ldots, \lambda_m, \sum_{k=1}^m \lambda_k = 1 \), then
\[
\text{Var}_D(A_1, A_2, A_3) \neq \sum_{k=1}^m \lambda_k \text{Var}_{P_k}(A_1, A_2, A_3).
\]

Let us use the Pauli matrices
\[
\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}
\]
to define \( A_1, A_2, A_3 \) in block-matrices in the following way
\[
A_1 := \begin{bmatrix} \sigma_1 & 0 \\ 0 & 0 \end{bmatrix}, \quad A_2 := \begin{bmatrix} \sigma_2 & 0 \\ 0 & 0 \end{bmatrix}, \quad A_3 := \begin{bmatrix} \sigma_3 & 0 \\ 0 & 0 \end{bmatrix},
\]
and $D := \text{Diag} \left( \frac{1}{2}, \frac{1}{2}, 0, \ldots, 0 \right)$. By the Lemma,

$$\text{Var}_D(A_1, A_2, A_3) = \sum_{k=1}^{m} \lambda_k \text{Var}_{P_k}(A_1, A_2, A_3)$$

if and only if $\text{Tr} P_k A_j = 0$ for every $k$ and $j$, but in this case we have $P_k^K = 0$ for $K = \text{range}(D)$, hence $D$ cannot be a convex combination of the $P_k$'s. Therefore, (10) holds.

The proof of the statement of the previous example is shorter if we use the Theorem. The only thing we have to observe is that

$$\dim \left( \text{span} \left\{ I^K, A_1^K, A_2^K, A_3^K \right\} \right) = (\dim K)^2$$

for $K = \text{range}(D)$.

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References


