Matrix variances with projections

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Abstract. The quantum variance of a self-adjoint operator depends on a density matrix whose particular example is a pure state (formulated by a projection). A general variance can be obtained from certain variances of pure states. This is very different from the probabilistic case.

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

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

when $D$ is a density matrix and $A \in M_n(\mathbb{C})$ is a self-adjoint operator [3], [4]. This is the straightforward analogy of the variance in probability theory [2]; a standard notation is $\langle A^2 \rangle - \langle A \rangle^2$ in both formalisms. It is rather different from probability theory that this variance can be strictly positive even in the case when $D$ has rank 1. If $D$ has rank 1, then it is an orthogonal projection and it is also called as pure state.

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 $D \mapsto \text{Var}_D(A)$:

$$\text{Var}_D(A) \geq \sum_i \lambda_i \text{Var}_{D_i}(A) \quad \text{if} \quad D = \sum_i \lambda_i D_i.$$

(Here $\lambda_i \geq 0$ and $\sum_i \lambda_i = 1$.)

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If we change the basis so that $D = \text{Diag}(p_1, p_2, \ldots, p_n)$, then we have

$$\text{Var}_D(A) = \sum_{i,j=1}^{n} \frac{p_i + p_j}{2} |A_{ij}|^2 - \left( \sum_{i=1}^{n} p_i A_{ii} \right)^2. \quad (2)$$

In the projection example $P = \text{Diag}(1, 0, \ldots, 0)$, formula (2) gives

$$\text{Var}_P(A) = \sum_{i \neq 1} |A_{1i}|^2$$

and this can be strictly positive.

**Theorem.** Let $D$ be a density matrix. Take all the decompositions such that

$$D = \sum_i q_i Q_i, \quad (3)$$

where $Q_i$ are pure states and $(q_i)$ is a probability distribution. Then

$$\text{Var}_D(A) = \sup \left( \sum_i q_i \left( \text{Tr} Q_i A^2 - (\text{Tr} Q_i A)^2 \right) \right), \quad (4)$$

where the supremum is over all decompositions (3).

The proof will be an application of matrix theory. The first lemma contains a trivial computation on block matrices.

**Lemma 1.** Assume that

$$D = \begin{bmatrix} D^\wedge & 0 \\ 0 & 0 \end{bmatrix}, \quad D_i = \begin{bmatrix} D_i^\wedge & 0 \\ 0 & 0 \end{bmatrix}, \quad A = \begin{bmatrix} A^\wedge & B \\ B^* & C \end{bmatrix}$$

and

$$D = \sum_i \lambda_i D_i, \quad D^\wedge = \sum_i \lambda_i D_i^\wedge.$$ 

Then

$$(\text{Tr} D^\wedge (A^\wedge)^2 - (\text{Tr} D^\wedge A^\wedge)^2) - \sum_i \lambda_i ((\text{Tr} D_i^\wedge (A^\wedge)^2 - (\text{Tr} D_i^\wedge A^\wedge)^2))$$

$$= (\text{Tr} D A^2 - (\text{Tr} D A)^2) - \sum_i \lambda_i ((\text{Tr} D_i A^2 - (\text{Tr} D_i A)^2)).$$

This lemma shows that if $D \in M_n(\mathbb{C})$ has a rank $k < n$, then the computation of a variance $\text{Var}_D(A)$ can be reduced to $k \times k$ matrices. The equality in (4) is rather obvious for a rank 2 density matrix and due to the previous lemma the computation will be with $2 \times 2$ matrices.
Lemma 2. For a rank 2 matrix D the equality holds in (4).

Proof. Due to Lemma 1 we can make the computation with $2 \times 2$ matrices. We can assume that

$$D = \begin{bmatrix} p & 0 \\ 0 & 1 - p \end{bmatrix}, \quad A = \begin{bmatrix} a_1 & b \\ \overline{b} & a_2 \end{bmatrix}. $$

Then

$$\text{Tr} \, DA^2 = p(a_1^2 + |b|^2) + (1 - p)(a_2^2 + |b|^2). $$

We can assume that

$$\text{Tr} \, DA = pa_1 + (1 - p)a_2 = 0. $$

Let

$$Q_1 = \begin{bmatrix} p & ce^{-i\varphi} \\ ce^{i\varphi} & 1 - p \end{bmatrix},$$

where $c = \sqrt{p(1 - p)}$. This is a projection and

$$\text{Tr} \, Q_1 A = a_1p + a_2(1 - p) + bce^{-i\varphi} + \overline{b}ce^{i\varphi} = 2c \text{Re} b e^{-i\varphi}. $$

We choose $\varphi$ such that $\text{Re} b e^{-i\varphi} = 0$. Then $\text{Tr} \, Q_1 A = 0$ and

$$\text{Tr} \, Q_1 A^2 = p(a_1^2 + |b|^2) + (1 - p)(a_2^2 + |b|^2) = \text{Tr} \, DA^2. $$

Let

$$Q_2 = \begin{bmatrix} p & -ce^{-i\varphi} \\ -ce^{i\varphi} & 1 - p \end{bmatrix}. $$

Then

$$D = \frac{1}{2} Q_1 + \frac{1}{2} Q_2$$

and we have

$$\frac{1}{2}(\text{Tr} \, Q_1 A^2 + \text{Tr} \, Q_1 A^2) = p(a_1^2 + |b|^2) + (1 - p)(a_2^2 + |b|^2) = \text{Tr} \, DA^2. $$

Therefore we have an equality.

We denote by $r(D)$ the rank of an operator $D$. The idea of the proof is to reduce the rank and the block-diagonal formalism will be used [1].

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Lemma 3. Let $D$ be a density matrix and $A = A^*$ be an observable. Assume the block-matrix forms

$$D = \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix}, \quad A = \begin{bmatrix} A_1 & A_2 \\ A_2^* & A_3 \end{bmatrix},$$

and $r(D_1), r(D_2) > 1$. We construct

$$D' := \begin{bmatrix} D_1 & X^* \\ X & D_2 \end{bmatrix}$$

such that

$$\text{Tr} DA = \text{Tr} D'A, \quad D' \geq 0, \quad r(D') < r(D).$$

Proof. The $\text{Tr} DA = \text{Tr} D'A$ condition is equivalent with $\text{Tr} XA_2 + \text{Tr} X^*A_2^* = 0$ and this holds if and only if $\text{Re} \text{Tr} XA_2 = 0$.

We can have unitaries $U$ and $W$ such that $UD_1U^*$ and $WD_2W^*$ are diagonal:

$$UD_1U^* = \text{Diag}(0, \ldots, 0, a_1, \ldots, a_k), \quad WD_2W^* = \text{Diag}(b_1, \ldots, b_l, 0, \ldots, 0)$$

where $a_i, b_j > 0$. Then $D$ has the same rank as the matrix

$$\begin{bmatrix} U & 0 \\ 0 & W \end{bmatrix} D \begin{bmatrix} U^* & 0 \\ 0 & W^* \end{bmatrix} = \begin{bmatrix} UD_1U^* & 0 \\ 0 & WD_2W^* \end{bmatrix},$$

the rank is $k + l$. A possible modification of this matrix is

$$Y := \begin{bmatrix} \text{Diag}(0, \ldots, 0, a_1, \ldots, a_{k-1}) & 0 & 0 & 0 \\ 0 & a_k & \sqrt{a_kb_1} & 0 \\ 0 & \sqrt{a_kb_1} & b_1 & 0 \\ 0 & 0 & 0 & \text{Diag}(b_2, \ldots, b_l, 0, \ldots, 0) \end{bmatrix}$$

$$= \begin{bmatrix} UD_1U^* & M \\ M & WD_2W^* \end{bmatrix}$$

and $r(Y) = k + l - 1$. So $Y$ has a smaller rank than $D$. Next we take

$$\begin{bmatrix} U^* & 0 \\ 0 & W^* \end{bmatrix} Y \begin{bmatrix} U & 0 \\ 0 & W \end{bmatrix} = \begin{bmatrix} D_1 & U^*MW \\ W^*MU & D_2 \end{bmatrix}$$

which has the same rank as $Y$. If $X := W^*MU$ is multiplied with $e^{i\alpha}$ ($\alpha > 0$), then the positivity condition and the rank remain. On the other hand, we can choose $\alpha > 0$ such that $\text{Re} \text{Tr} e^{i\alpha}X_1A_2 = 0$. Then $X := e^{i\alpha}X_1$ is the matrix we wanted.
**Lemma 4.** Let $D$ be a density matrix of rank $m > 1$ and $A = A^*$ be an observable. We claim the existence of a decomposition

\[ D = pD_- + (1 - p)D_+, \]

such that $r(D_-) < m$, $r(D_+) < m$, and

\[ \text{Tr } AD_+ = \text{Tr } AD_- = \text{Tr } DA. \]

**Proof.** By unitary transformation we can get to the formalism of the previous lemma:

\[ D = \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix}, \quad A = \begin{bmatrix} A_1 & A_2 \\ A_2^* & A_3 \end{bmatrix}. \]

We choose

\[ D_+ = D' = \begin{bmatrix} D_1 & X^* \\ X & D_2 \end{bmatrix}, \quad D_- = \begin{bmatrix} D_1 & -X^* \\ -X & D_2 \end{bmatrix}. \]

Then

\[ D = \frac{1}{2} D_- + \frac{1}{2} D_+ \]

and the requirements $\text{Tr } AD_+ = \text{Tr } AD_- = \text{Tr } DA$ also hold.

**Proof of the Theorem.** For rank-2 states, it is true because of Lemma 2. Any state with a rank larger than 2 can be decomposed into the mixture of lower rank states, according to Lemma 4, that have the same expectation value for $A$, as the original state has. The lower rank states can then be decomposed into the mixture of states with an even lower rank, until we reach rank-2 states. Thus, any state $D$ can be decomposed into the mixture of

\[ D = \sum p_k Q_k \]

such that $\text{Tr } A Q_k = \text{Tr } AD$. Hence the statement of the theorem follows.

The above theorem has been included in [5] already, but the strictly mathematical argument and the matrix formalism appear here.
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