Totally Positive Density Matrices and Linear Preservers

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TOTALLY POSITIVE DENSITY MATRICES
AND LINEAR PRESERVERS

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Abstract. The intersection between the set of totally nonnegative matrices, which are of interest in many areas of matrix theory and its applications, and the set of density matrices, which provide the mathematical description of quantum states, are investigated. The single qubit case is characterized, and several equivalent conditions for a quantum channel to preserve the set in that case are given. Higher dimensional cases are also discussed.

Key words. Totally nonnegative matrix, Totally positive matrix, Density matrix, Linear preservers, Completely positive map, Quantum channel.

AMS subject classifications. 15A86, 15B48, 81P45.

1. Introduction and background. Density matrices are fundamental objects of study in quantum mechanics and quantum information theory [10]. On the other hand, totally positive and totally nonnegative matrices [6] have been studied for almost eighty years in the matrix theory community for a variety of theoretical and application motivated reasons. In this short paper, we bring together these topics for the first time and ask a pair of basic questions: What do matrices with both features look like, and, can we characterize the linear maps, in particular the completely positive maps, that preserve this set? We present a complete answer, both computationally and geometrically, for the single qubit case and we discuss higher dimensional cases.

We begin by presenting requisite background material, written for both matrix theorists and quantum information theorists.

1.1. Totally positive matrices. Let $M$ be any $m$ by $n$ real matrix. A real number is a minor of $M$ if it is the determinant of any square submatrix of $M$. The matrix $M$ is said to be totally positive (resp. totally nonnegative) if all of its minors are positive (resp. nonnegative). Interestingly, it was a physical application, namely the study of oscillations in mechanical systems, which led Gantmacher and Krein to first study these classes of matrices in the 1930’s [8]. The theory of totally nonnegative matrices has further developed over the years and has found applications.
in combinatorics, approximation theory, stochastic processes and quantum groups amongst other areas. We point the reader to the references \[1, 5–7, 9, 12\] as entrance points into the literature on totally nonnegative matrices. Some authors use “totally positive” where we have used “totally nonnegative”, and “strictly totally positive” (STP) for our “totally positive”. We will abbreviate “totally nonnegative” by TN and “totally positive” by TP.

In order to refer to particular minors of a matrix, we will use the following notation:

**Notation 1.** Let \( I = \{i_1, \ldots, i_k\} \subseteq \{1, 2, \ldots, n\} \), and let \( J = \{j_1, \ldots, j_k\} \subseteq \{1, 2, \ldots, m\} \), where \( n \) is the number of rows and \( m \) the number of columns of a matrix \( A \), and \( k \leq \min\{n, m\} \). We also take \( I \) and \( J \) to be ordered in increasing order. Then \([A]_{i_1, i_2, \ldots, i_k|j_1, j_2, \ldots, j_k}\) refers to the submatrix of \( A \) comprising rows \( i_1, i_2, \ldots, i_k \) and columns \( j_1, j_2, \ldots, j_k \). We also write for this matrix \( A_{i_1, i_2, \ldots, i_k|j_1, j_2, \ldots, j_k}\).

**Proposition 1.** Let \( A \in \mathbb{R}^{n \times n} \) be TP. Then the eigenvalues of \( A \), \( \{\lambda_i\}^n_{i=1} \) are all distinct positive real numbers.

This result also has a converse:

**Proposition 2.** Let \( \lambda_1 > \lambda_2 > \lambda_3 > \cdots > \lambda_n > 0 \) be a list of distinct positive real numbers. Then there exists an \( n \times n \) TP matrix with \( \{\lambda_i\}^n_{i=1} \) as its eigenvalues.

**1.2. Density matrices.** A density matrix represents a quantum state; specifically, a density matrix \( \rho \) is a positive semi-definite matrix with \( tr(\rho) = 1 \). Linear maps that preserve density matrix structure are called quantum channels, and the mathematical formalism for such maps is well-known \[10,11\].

A linear map \( \Phi : \mathbb{C}^{n \times n} \to \mathbb{C}^{n \times n} \) is said to be positive if it preserves the set of positive semi-definite matrices; i.e., if \( \rho \in \mathbb{C}^{n \times n} \) is positive semi-definite, then \( \Phi(\rho) \) is positive semi-definite as well. \( \Phi \) is said to be \( k \)-positive if \( id_k \otimes \Phi \) is positive; that is, if the \( k \times k \) identity map tensored with \( \Phi \) preserves positive-semidefiniteness on \( \mathbb{C}^{nk \times nk} \). Finally, a map is completely positive if it is \( k \)-positive for all \( k \). As a consequence of Stinespring’s dilation theorem \[14\] in the finite-dimensional case, we know that \( \Phi \) is completely positive if and only if there exist matrices \( K_i \) such that \( \Phi(\rho) = \sum_{i=1}^{n} K_i \rho K_i^\dagger \). The operators \( K_i \) are called the Kraus operators of the map \( \Phi \). Another representation of a CP map is in terms of its Choi matrix, which is the
matrix

\[ C_{\Phi} := \sum_{i,j} E_{ij} \otimes \Phi(E_{ij}), \]

where \( E_{ij} \) is the matrix with a 1 in the \( i, j \) entry and 0’s elsewhere (\( E_{ij} = |i\rangle\langle j| \) in the Dirac notation mentioned below). A linear map \( \Phi \) is CP if and only if \( C_{\Phi} \) is positive [3]. A quantum channel is a completely positive trace-preserving (CPTP) map.

Lastly, we mention the notion of the dual to a CP map. The Hilbert-Schmidt inner product on the space of \( M_{n}(\mathbb{C}^n) \) is given by \((A,B) = \text{tr}(A^\dagger B)\). The dual of a map \( \Phi \) is the dual in this inner product: \( \Phi^\dagger \) is defined so that \((\Phi(A),B) = (A,\Phi^\dagger(B))\); in terms of the Kraus operators, if \( \Phi(\cdot) = \sum_i K_i \cdot K_i^\dagger \) then \( \Phi^\dagger(\cdot) = \sum_i K_i^\dagger \cdot K_i \).

1.3. The Bloch sphere. \( 2 \times 2 \) density matrices can be represented as follows:

The Pauli matrices

\[
I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

determine all \( 2 \times 2 \) (single qubit) density matrices via the equation

\[
\rho = \frac{1}{2}(I_2 + r_1\sigma_x + r_2\sigma_y + r_3\sigma_z)
\]

with \( r_1^2 + r_2^2 + r_3^2 \leq 1 \), which ensures positive semi-definiteness. Hence, the single qubit density matrices can be identified with the points \((r_1, r_2, r_3)\) in the unit sphere, which is called the Bloch sphere representation: on its surface are the rank-one density operators, or pure states; interior points correspond to mixed states. Under this identification, \( E_{11} = \frac{1}{2}(I_2 + Z) \) is identified with the north pole of the sphere, \( \frac{1}{2}J_2 = \frac{1}{2}(I_2 + X) \) with the point \((1,0,0)\) on the Bloch sphere, and \( \frac{1}{2}(J_2 + Y) \) with the point \((0,1,0)\).

We also recall the Dirac bra-ket notation: A vector in \( \mathbb{C}^n \) is identified with a ket, so that the state \( \psi \) is written \( |\psi\rangle \). Elements of the dual space are denoted by bras, written \( \langle \psi | \). Outer product operators are written in this notation as \( |\phi\rangle\langle \psi | \), which acts on a vector \( |v\rangle \) by projecting onto \( |\phi\rangle \) as \( |\phi\rangle\langle \psi |v\rangle = \langle \psi |v\rangle|\phi\rangle \). We mention lastly that tensor products between vectors are written by conjunction, so that \( |\psi\rangle \otimes |\phi\rangle \) is written either as \( |\psi\rangle|\phi\rangle \) or even \( |\psi\phi\rangle \).

2. Single qubit totally positive density matrices. In this section, we investigate those single qubit density matrices that are also totally positive matrices. As total positivity is heavily basis dependent (recall that any list of distinct positive numbers is the eigenvalue set of some TP matrix), we will fix a basis in this case the computational basis \( \{e_1, e_2, \ldots, e_n\} \) or \( e_i = |i\rangle \) in Dirac notation. Note that any symmetric totally nonnegative matrix is also a positive semidefinite matrix.
Observe the matrices \( \frac{1}{2}(I + Z), \frac{1}{2}(I - Z), \frac{1}{2}(I + X) \) are all TN density matrices, corresponding to the points \((0, 0, 1), (0, 0, -1)\) and \((1, 0, 0)\) on the Bloch sphere.

**Lemma 1.** A symmetric matrix with positive entries is totally determined by its principal minors of size \(1 \times 1\) and \(2 \times 2\).

**Proof.** This follows easily from the fact that

\[
\]

In particular, by always choosing the positive square root of this quantity we obtain a symmetric matrix with positive entries. \(\Box\)

An obvious necessary condition on a real symmetric TP matrix is that

\[
A[j|i,j] < a_{ii}a_{jj}.
\]

For \(2 \times 2\) matrices, we only have two free parameters: the \(a_{11}\) entry \(a\), and the determinant \(\det(A)\). By choosing \(0 \leq a_{11} \leq 1\) and \(\det(A) \leq a(1 - a)\) we obtain a symmetric TP density matrix

\[
A = \left( \frac{a}{\sqrt{a(1-a) - \det(A)}} \right) \left( \begin{array}{cc} \frac{1}{2} & \frac{1}{2} + r_3 - r_2 i \\ r_2 + ir_3 & 1 - r_3 \end{array} \right).
\]

**Proposition 3.** The \(2 \times 2\) TN density matrices are those density matrices such that \(r_1^2 + r_2^2 \leq 1\), \(r_1 \geq 0\), and \(r_2 = 0\). The TP matrices are those for which \(r_1 \neq 0\) and \(r_1^2 + r_2^3 < 1\). This corresponds to a closed semicircular region inside the Bloch sphere.

**Proof.** Let \(A\) be a \(2 \times 2\) TN density matrix. Then from the Bloch sphere representation,

\[
A = \frac{1}{2} \left( \begin{array}{cc} 1 + r_3 & r_3 - ir_2 \\ r_2 + ir_3 & 1 - r_3 \end{array} \right).
\]

Thus, \(r_2 = 0\) is necessary for \(A\) to be real, \(r_1 \geq 0\) is necessary for \(A\) to have nonnegative entries \((r_1 \neq 0\) if \(A\) is to have positive entries), and \(r_1^2 + r_2^3 \leq 1\) is necessary for \(A\) to be a density matrix.

For sufficiency, let \(A\) have the form above, subject to the mentioned conditions. Clearly, the matrix is real and symmetric, and its off-diagonal entries are nonnegative. Since \(r_2^3 \leq 1\), we have \(1 \pm r_3 \geq 0\), and thus, \(A\) has all positive entries. The trace is easily computed to be 1. Moreover,

\[
\det(A) = \frac{1}{4}[(1 + r_3)(1 - r_3) - r_2^2] = \frac{1}{4}(1 - r_3^2 - r_1^2) \geq 0,
\]

since \(r_4^2 + r_3^2 \leq 1\). If \(r_1^2 + r_3^2 < 1\), then the determinant is strictly positive. Thus, \(A\) is symmetric, trace 1, and all of its minors are nonnegative, and so it must have
3. Quantum channel preservers of $TN$ density matrices. In this section, we investigate the structure of those single qubit CPTP maps that preserve the set of $TN$ density matrices.

**Lemma 2.** The single qubit $TN$ density matrices are the convex hull of the rank-one $TN$ density matrices.

**Proof.** Geometrically, the $TN$ density matrices lie in the half-circle bounded by the line from the north pole to the south pole of the Bloch sphere, and the semi-circle consisting of density matrices of the form

\[
\begin{pmatrix}
a & a(1-a) \\ \sqrt{a(1-a)} & 1-a
\end{pmatrix}.
\]

That is, the rank-one $TN$ density matrices, since such a matrix may be written as $|v\rangle\langle v|$ where $|v\rangle = \sqrt{a}|0\rangle + \sqrt{1-a}|1\rangle$. The lemma corresponds to the observation that, since the north and south poles, corresponding to the matrices $\frac{1}{2}(I+Z), \frac{1}{2}(I-Z)$ are also rank-ones, then the boundary of the semi-circle consists of either rank-ones, or mixtures of these two rank-one operators. Since the semi-circle is convex, all other points in the semi-circle may be written as convex combinations of points on the boundary.

Thus, in order to identify the CPTP maps that take the set of $TN$ matrices into themselves, it suffices to find those maps which map rank-one $TN$ matrices to $TN$ matrices, with preservation of rank-two $TN$ density matrices following from linearity. The following theorem gives multiple equivalent solutions to this problem, in terms of testable conditions on the Choi matrix for the map.

**Theorem 1.** Let $\Phi : \mathbb{C}^{2\times2} \to \mathbb{C}^{2\times2}$ be a CPTP map with Choi matrix $C_\Phi = (c_{ij})_{1\leq i,j \leq 4}$. The following are equivalent:

1. $\Phi$ preserves the set of $TN$ density matrices.
2. $\Phi$ maps the rank-one $TN$ density matrices into the $TN$ density matrices.
3. The matrix $\begin{pmatrix} c_{12} & c_{14} + c_{23} \\ c_{14} + c_{23} & c_{34} \end{pmatrix}$ is copositive.
4. The submatrix $C_\Phi[1, 2|3, 4]$ of $C_\Phi$ is copositive.
5. The following inequalities are satisfied:
   \[ c_{12}, c_{34} \geq 0 \quad \text{and} \quad c_{14} + c_{23} \geq -\sqrt{c_{12}c_{34}}. \]
6. The matrix $\Phi^\dagger(E_{12}) = \Phi^\dagger(|0\rangle\langle 1|)$ is co-positive.

Before proceeding, we recall a notion from matrix theory that arises in the result: a variant of matrix positivity referred to as copositivity. A matrix $A$ is copositive if $\langle x|Ax|x \rangle \geq 0$ for all vectors $|x\rangle \in \mathbb{R}^n$ that only have nonnegative components.
Proof. For the equivalence of the first two conditions, (2) follows from (1) a fortiori, and (2) \(\Rightarrow\) (1) follows from the fact that the TN density matrices are the convex hull of the rank-one TN density matrices, together with the linearity of \(\Phi\).

To see the equivalence (2) \(\Leftrightarrow\) (3): Let \(|v\rangle\langle v| = \begin{pmatrix} a^2 & ab \\ ab & b^2 \end{pmatrix}\) be a rank-one TN density matrix, and let \(C_\Phi\) be as above. Then
\[
\Phi(|v\rangle\langle v|) = a^2 \begin{pmatrix} c_{11} & c_{12} \\ c_{12} & c_{22} \end{pmatrix} + ab \begin{pmatrix} 2c_{13} & c_{14} + c_{23} \\ c_{14} + c_{23} & 2c_{24} \end{pmatrix} + b^2 \begin{pmatrix} c_{33} & c_{34} \\ c_{34} & c_{44} \end{pmatrix}.
\]

Since \(\Phi\) is CPTP, \(\Phi(|v\rangle\langle v|)\) must have positive diagonal entries and positive determinant, thus the only other condition that must be satisfied for \(\Phi(|v\rangle\langle v|)\) to be TN is for its off-diagonal entries to be nonnegative. Hence, we require for all \(a, b \geq 0\) that
\[a^2 c_{12} + ab(c_{14} + c_{23}) + b^2 c_{34} \geq 0.\]
We re-write this as
\[
(a b) \begin{pmatrix} c_{12} \\ c_{14} + c_{23} \\ c_{34} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \geq 0
\]
for all \(a, b \geq 0\), which is exactly the definition of co-positivity. As a side note, observe that the last expression is a quadratic form in \(a, b\), so that positivity of this matrix may be phrased as a problem in semi-algebraic geometry: we require that the homogeneous polynomial \(a^2 c_{12} + ab(c_{14} + c_{23}) + b^2 c_{34}\) is nonnegative for all \(a, b \geq 0\). For the other direction of this equivalence, we can reverse the proof and note that any Choi matrix with this property will necessarily map the set of rank-one TN density matrices to TN density matrices, and thus by convexity and linearity, must preserve all \(2 \times 2\) TN density matrices.

To establish the equivalence with (4), observe that the matrix
\[
\begin{pmatrix} c_{12} & c_{14} + c_{23} \\ c_{14} + c_{23} & c_{34} \end{pmatrix} = (M + M^T),
\]
where \(M\) is the \([1, 2|3, 4]\) submatrix of \(C_\Phi\). However, \(M\) is co-positive whenever \(M + M^T\) is, and so an equivalent characterization is that \(C_\Phi[1, 2|3, 4]\) be co-positive.

To see (5), we note that for \(n \times n\) matrices where \(n \leq 5\), there is a useful characterization of co-positivity: an \(n \times n\) matrix is co-positive when it can be written as the sum of a positive semi-definite matrix and a matrix with nonnegative entries. Since in our case the matrix in question is symmetric, the condition that the matrix in condition (4) is co-positive is thus equivalent to the statement that \(c_{12}, c_{34} \geq 0\) and \(c_{14} + c_{23} \geq -\sqrt{c_{12} c_{34}}\).

Condition (6) can be seen as equivalent to (2) via consideration of the Kraus operator decomposition and the low-dimensional description of co-positivity mentioned above. Indeed, let \(\Phi\) have a Kraus decomposition \(\Phi(\rho) = \sum_i K_i \rho K_i^\dagger\). The condition that the off-diagonal entries of \(\Phi(|v\rangle\langle v|)\) be positive is the condition that
\[ \sum_{i} e_{1}^{\dagger} K_{i} v e_{2} v^T K_{i}^{\dagger} e_{2} \geq 0, \]

or, using the Dirac notation

\[ \sum_{i} \langle 0 | K_{i} | v \rangle \langle v | K_{i}^{\dagger} | 1 \rangle \geq 0. \]

The Dirac notation makes it clear that \( \langle 0 | K_{i} | v \rangle \) and \( \langle v | K_{i}^{\dagger} | 1 \rangle \) are both scalars, so they commute:

\[ \sum_{i} \langle v | K_{i}^{\dagger} | 1 \rangle \langle | K_{i} | v \rangle = \langle v | \left( \sum_{i} K_{i}^{\dagger} E_{ij} K_{i} \right) | v \rangle \geq 0 \]

for all \( |v\rangle \in \mathbb{R}^2 \). This condition is equivalent to the statement that the matrix \( \sum_{i} K_{i}^{\dagger} E_{12} K_{i} = \Phi^{\dagger}(E_{12}) \) is co-positive. \( \square \)

### 4. Concluding remarks.

The restriction to totally positive density matrices may seem in some ways unnatural from a quantum information point of view, since total positivity requires real entries for our matrix. We wish to note, then, that real density matrices or “rebits” have been considered in the context of quantum information, see [2,4,13,15] for some studies on the role and uses of rebits in quantum information.

While there are many physical and application oriented reasons for investigating density matrices and totally positive matrices separately, our motivation for considering them here was naively mathematical. We simply asked whether there is a structure that describes matrices with both properties, and if completely positive maps that preserve these matrices have structure themselves. We have given a comprehensive answer to these questions for the single qubit case. Looking toward the \( n \geq 3 \) cases the qubit case can be used as motivation, but there are immediate challenges one confronts in higher dimensions. Probably the main challenge is that unlike the \( n = 2 \) case, neither the TN matrices nor even the TN density matrices form a convex set. A simple example of the latter fact is the pair of matrices:

\[ A = \frac{1}{11} \begin{pmatrix} 2 & 4 & 1 \\ 4 & 15 & 2 \\ 1 & 4 & 2 \end{pmatrix}, \quad B = \frac{1}{17} \begin{pmatrix} 17 & 4 & 15 \\ 4 & 15 & 4 \\ 15 & 4 & 17 \end{pmatrix}. \]

The lower left minor of their average is negative, even though each individually is TN. Another fact that may be relevant to the difficulty of extending this analysis to the case \( n \geq 3 \) is that any \( 2 \times 2 \) TN matrix can be symmetrized by some diagonal matrix to a symmetric, and thus positive semidefinite matrix, a fact which is not true in higher dimensions. Of course, the problem could be made more tractable and still interesting by adjusting hypotheses. For instance, even in the case of the more general problem of characterizing linear preservers of TN matrices in low-dimensions, relaxing the constraint that the matrices preserved be density matrices could simplify the problem. There appear to be potentially interesting problems to consider here, and this work should be viewed as an invitation to interested researchers to explore them.
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