DILATION THEORETIC PARAMETRIZATIONS OF POSITIVE MATRICES WITH APPLICATIONS TO QUANTUM INFORMATION

M. C. TSENG AND V. RAMAKRISHNA
DEPARTMENT OF MATHEMATICAL SCIENCES
UNIVERSITY OF TEXAS AT DALLAS

Abstract. In this note, dedicated to the memory of Professor Tiberiu Constantinescu, we discuss the applications of two parametrizations of positive matrices to issues in quantum information theory. The first, which we propose be dubbed the Schur-Constantinescu parametrization, is used in a twin fashion to construct examples of separable states in arbitrary dimensions. The second, called the Jacobi parametrization, is used to describe quantum states in dimension two, as an alternative to the Bloch sphere representation.

1. Introduction

Tiberiu Constantinescu, mathematician, mentor and colleague par excellence, was interested in the rapidly developing field of quantum information theory during the last few years of his life, [7, 8]. In particular in [8], several useful applications of the Schur parameters to quantum information theory were presented. Thus, for instance, the fact that the Schur parametrization automatically yields the Cholesky factorization of the positive matrix in question implies that a Kraus operator representation for quantum channels can be directly found without any need for spectral factorization. In particular, viewing a quantum state as a channel with one-dimensional input space, one can thereby find an ensemble representation for quantum states, which is different from that provided by the state’s spectral decomposition. Similarly, the fact that the determinant of a positive matrix can be directly found from its Schur parameters is useful in computing some entropic quantities. The Schur parameters were also shown to yield a simply verified necessary and sufficient condition for purity (i.e., for the quantum state to have rank one). This is particularly interesting since there have been several attempts to extend the Bloch sphere condition for pure states in dimension two, [1, 12, 14], to higher dimensions. Whilst necessary and sufficient conditions can be stated, these conditions are typically difficult to analyse. In this note, with a view towards further popularizing this parametrization, we show how it can be used to construct examples of separable states in a non-ad-hoc fashion.

Remark 1. Whilst several researchers have made impressive contributions to the field of Schur analysis (see [2, 6] and the extensive bibliography therein), it is our humble opinion that it was Tiberiu Constantinescu that brought forth the versatility of this
field to the maximum. Thus, we propose that these parameters be dubbed the Schur-Constantinescu parameters (SC, for short), at least for the purposes of this note.

In his most recent work, Tibi and his student developed a second parametrization of positive matrices called the Jacobi parametrization, [9, 10], which loosely speaking is to positive Hankel matrices what the SC parameterization is to positive Toeplitz matrices. This parametrization also yields the Cholesky factorization and the determinant of the positive matrix being parametrized, and thus would yield applications similar to those in [8]. However, unlike the SC parametrization, the Jacobi parametrization lacks an inheritance principle (see [9]), and thus its utility, pending further investigation, seems limited in comparison to the SC parametrization. Instead of reporting results on Kraus representations etc., analogous to those in [8], we will restrict ourselves to showing how qubit states can be described via the Jacobi parametrization. At this point we do not have a simple criterion for purity in higher dimensions analogous to that produced by the SC parametrization (and this is, in part, due to the lack of this inheritance principle), and thus we will restrict ourselves to qubit states in this note.

Partly with a view towards convincing researchers in quantum information theory of the utility of the SC and Jacobi parametrization, and partly out of deference to Tibi’s abiding dedication to didaction, we will present a “user friendly” informal derivation of these two parametrizations. We hope that this will stimulate novices in the field of Schur analysis (as indeed, both authors of this note themselves are) to peruse Tibi’s innumerable contributions to this field.

The balance of this note is organized as follows. In the next section the SC parametrization is presented. The next section contains our results on separability. The fourth section presents the Jacobi parametrization. The fifth describes the Jacobi picture of qubit states. The final section offers conclusions.

2. SC PARAMETRIZATION

We only provide the essential results required, together with informal proofs where possible - the definitive and comprehensive treatment of SC parameters is given in [6]. In the following discussion, $\mathcal{H}$, with subscripts, will denote a Hilbert space. $\mathcal{L}(\mathcal{H}_i, \mathcal{H}_j)$ is the space of bounded operators from $\mathcal{H}_i$ to $\mathcal{H}_j$ and $\mathcal{L}(\mathcal{H}, \mathcal{H}) = \mathcal{L}(\mathcal{H})$.

Let

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{12}^* & A_{22} \end{bmatrix} \in \mathcal{L}(\mathcal{H}_1 \oplus \mathcal{H}_2)$$

be a positive semidefinite operator matrix whose entries are bounded operators, that is

$$\langle \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}, A \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} \rangle_{\mathcal{H}_1 \oplus \mathcal{H}_2} \geq 0$$
Theorem 1. To summarize the above calculations:

For all $h_1 \in \mathcal{H}_1$ and $h_2 \in \mathcal{H}_2$. Clearly the diagonal blocks themselves are then positive. We will show that there exists an unique contraction $\Gamma \in \mathcal{L}(\mathcal{H}_2, \mathcal{H}_1)$ such that $A_{12} = A_{12}^* \Gamma A_{22}^\frac{1}{2}$. To this end, assume for the moment that both $A_{11}$ and $A_{22}$ are invertible. Then a Frobenius-Schur identity holds:

\[
A = \begin{bmatrix} A_{11} & A_{12} \\ A_{12}^* & A_{22} \end{bmatrix} = \begin{bmatrix} I & 0 \\ A_{12}^* A_{11}^{-1} & I \end{bmatrix} \cdot \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} - A_{12}^* A_{11}^{-1} A_{12} \end{bmatrix} \cdot \begin{bmatrix} I & A_{11}^{-1} A_{12} \\ 0 & I \end{bmatrix}.
\]

We deduce that $A$ is positive iff its Schur complement

\[
A_{22} - A_{12}^* A_{11}^{-1} A_{12} = A_{22}^\frac{1}{2} (I - A_{22}^{-\frac{1}{2}} A_{12}^* A_{11}^{-1} A_{12} A_{22}^{-\frac{1}{2}}) A_{22}^{-\frac{1}{2}}
\]

is positive, which implies

\[
I - A_{22}^{-\frac{1}{2}} A_{12}^* A_{11}^{-1} A_{12} A_{22}^{-\frac{1}{2}} \geq 0.
\]

The above can then be written as $(I - \Gamma^* \Gamma) \geq 0$. In other words, the suitable contraction is $\Gamma = A_{11}^{-\frac{1}{2}} A_{12} A_{22}^{-\frac{1}{2}}$.

For the more general case that $A_{11}$ and $A_{22}$ are not invertible, consider the sequences $\{\alpha_n = A_{11} + \frac{1}{n}\}$ and $\{\beta_n = A_{22} + \frac{1}{n}\}$. By the spectral mapping theorem for self adjoint operators, $\alpha_n$ and $\beta_n$ are invertible for all $n$. Therefore there exist contractions $\{\Gamma_n\}$ with $A_{12} = \alpha_n^\frac{1}{2} \Gamma_n \beta_n^\frac{1}{2}$. Since the unit ball in $\mathcal{L}(\mathcal{H}_2, \mathcal{H}_1)$ is compact in the weak operator topology, $\Gamma_n$ converges to some contraction $\Gamma$ weakly. We can compute directly, for all $h_1 \in \mathcal{H}_1$ and $h_2 \in \mathcal{H}_2$,

\[
\langle h_1, A_{11}^\frac{1}{2} \Gamma A_{22}^\frac{1}{2} h_2 \rangle_{\mathcal{H}_1} = \lim_n \langle h_1, A_{11}^\frac{1}{2} \Gamma_n A_{22}^\frac{1}{2} h_2 \rangle_{\mathcal{H}_1} = \lim_n \langle h_1, \alpha_n^\frac{1}{2} \Gamma_n \beta_n^\frac{1}{2} h_2 \rangle_{\mathcal{H}_1} = \langle h_1, A_{12} h_2 \rangle_{\mathcal{H}_1}.
\]

To summarize the above calculations:

**Theorem 1.** The operator matrix

\[
A = \begin{bmatrix} A_{11} & A_{12} \\ A_{12}^* & A_{22} \end{bmatrix}
\]

with $A_{ii} \geq 0$ is positive iff there exists a contraction $\Gamma$ such that $A_{11}^\frac{1}{2} \Gamma A_{22}^\frac{1}{2} = A_{12}^2$.

In the argument given, the unique positive square roots of $A_{11}$ and $A_{22}$ were used. In fact $A_{11}^\frac{1}{2}$ and $A_{22}^\frac{1}{2}$ can be replaced by any operator $L_1$ and $L_2$ satisfying $A_{11} = L_1^* L_1$ and $A_{22} = L_2^* L_2$.

We next explain the crucial link between the these contractions and the Cholesky factorization. For a contraction $\Gamma$, we introduce its defect operator $D_{\Gamma} = (I - \Gamma^* \Gamma)^{\frac{1}{2}}$. Since $\Gamma(I - \Gamma^* \Gamma) = (I - \Gamma^* \Gamma)^{\frac{1}{2}}$, it follows that $\Gamma D_{\Gamma} = D_{\Gamma} \Gamma$. The Frobenius-Schur identity leads to a Cholesky factorization of $2 \times 2$ operator matrices:
\[ A = \begin{bmatrix} L_1^* L_1 & L_1^* \Gamma L_2 \\ L_2^* \Gamma L_1 & L_2^* L_2 \end{bmatrix} = \begin{bmatrix} L_1^* & 0 \\ L_2^* \Gamma & L_2^* D \Gamma \end{bmatrix} \begin{bmatrix} L_1 & \Gamma L_2 \\ 0 & D \Gamma L_2 \end{bmatrix}. \]

With a view towards extending this to operator matrices of size larger than 2 \times 2, we first present the following result:

**Theorem 2.** An operator \( T = [T_1 \ T_2 \ \cdots \ T_n] \in \mathcal{L}(\oplus_i^n \mathcal{H}_i, \mathcal{H}) \) is a contraction iff \( T_1 = \Gamma_1 \) is a contraction and there exist \( \Gamma_i \) such that \( T_i = D_{\Gamma_1} \Gamma_2 \cdots \Gamma_{k-1} \Gamma_k \).

The proof follows by induction and is omitted.

Having a characterization of row contractions, we now examine the 3 \times 3 case. From theorem 1, an arbitrary positive \( A \in \mathcal{L}(\oplus_i^3 \mathcal{H}_i) \) is of the form:

\[
A = \begin{bmatrix} L_1^* L_1 & L_1^* \Gamma_{12} L_2 & B \\ L_2^* \Gamma_{12} L_1 & L_2^* L_2 & L_2^* \Gamma_{23} L_3 \\ B^* & L_3^* \Gamma_{23} L_2 & L_3^* L_3 \end{bmatrix}
\]

where the \( \Gamma_{ij} \)'s are contractions. We will show that \( B \) can be parametrized by contractions. Again from theorem 1,

\[
[L_1^* \Gamma_{12} L_2 \ B] = L_1^* \cdot \Lambda \cdot \begin{bmatrix} L_2 & \Gamma_{23} L_3 \\ 0 & D_{\Gamma_{23}} L_3 \end{bmatrix}
\]

where \( \Lambda \in \mathcal{L}(\mathcal{H}_2 \oplus \mathcal{H}_3, \mathcal{H}_1) \) is a contraction. By theorem 2, we can assume

\[
\Lambda = [\Lambda_1 \ D_{\Lambda_1} \Lambda_2]
\]

for contractions \( \Lambda_i \). Evidently we can choose \( \Lambda_1 = \Gamma_{12} \) and let \( \Lambda_2 = \Gamma_{13} \) to obtain

\[
B = L_1^* (\Gamma_{12} \Gamma_{23} + D_{\Gamma_{12}} \Gamma_{13} D_{\Gamma_{23}}) L_3^*.
\]

This can be generalized to positive operator matrices of arbitrary size. Let \( A = [A_{ij}]_{ij} \in \mathcal{L}(\oplus_i^n \mathcal{H}_i) \) be positive. The SC parametrization of \( A \) can be calculated recursively as follows:

i) \[ \begin{bmatrix} A_{n-1,n-1} & A_{n-1,n} \\ A_{n,n-1} & A_{n,n} \end{bmatrix} \] is positive and can be parametrized according to the 2 \times 2 case.

ii) For \( 1 \leq k \leq n - 2 \), the SC parametrization of

\[
\begin{bmatrix}
A_{k,k} & A_{k,k+1} & \cdots & A_{k,n} \\
A_{k+1,k} & A_{k+1,k+1} & \cdots & A_{k+1,n} \\
\vdots & \vdots & \ddots & \vdots \\
A_{n,k} & A_{n,k+1} & \cdots & A_{n,n}
\end{bmatrix}
\]

is calculated by first considering

\[
\begin{bmatrix}
A_{k+1,k+1} & \cdots & A_{k+1,n} \\
\vdots & \ddots & \vdots \\
A_{n,k+1} & \cdots & A_{n,n}
\end{bmatrix} = L_{k+1,k+1}^* L_{k+1,k+1}.
\]
where $L_{k+1}$ is the Cholesky factor calculated in the previous step.

Then put \([A_{k,k+1} \cdots A_{k,n}] = A_{k,k}^{-\frac{1}{2}}R_kL_{k+1}\) with $R_k$ being the corresponding row contraction.

The contractions $\Gamma_{ij}, j > i$ are called the Schur-Constantinescu (SC) parameters of the matrix $A$. If the entries of $A$ are scalars these are numbers in the unit disc. For a positive matrix with scalar entries we adopt the convention that $\Gamma_{ij} = 0$ whenever $A_{ii}A_{jj} = 0$ (see [8]). Whilst applying the above iterative procedure leads to long expressions for the $\Gamma_{ij}$, these formulae can be easily represented via a transmission line diagram (this is also closely related to the notion of Dyck paths, see [6, 9]), and thus can be easily written down. The figure below illustrates this for the $4 \times 4$ case. This gives an easy way to compute the parameters. Each entry of the positive semidefinite \(\{A_{ij}\}\) corresponds to those paths in the diagram that start from $L_{jj}$ and end at $L_{ii}^*$. For example, each path from $L_{33}$ to $L_{11}^*$ describes to a summand in the parametrization of $A_{13}$.

**Figure 1.** Cholesky factorization for $4 \times 4$ positive matrices

**Remark 2.** The terminology scalar matrix will be used in the sequel to indicate that a certain matrix is being thought of as having entries which are $1 \times 1$, in order to distinguish it from the general operator matrix case. It should not be confused with a matrix of the form $\lambda I, \lambda \in \mathbb{C}$.

### 3. SC parameters and Separability

We assume that the notions of density matrix, pure states (i.e, rank one density matrices), positive preserving, complete positivity, Kraus representations and Choi matrix are known to the reader (see [1, 12]). When there is no chance of confusion, we will refer to a positive preserving map, $\Phi$ simply as positive.

A quantum state on a tensor product of two Hilbert spaces is said to be separable if it can be expressed as a convex combination of product states. Characterizing separability is an important problem, since its violation, viz., the phenomenon of quantum
entanglement plays an essential role in quantum information protocols. For $2 \otimes 2$ and $2 \otimes 3$ states there is a simple necessary and sufficient condition for separability, the so-called Peres-Horodecki PPT condition, [13, 14]. For other dimensions the only known necessary and sufficient conditions are difficult to work with in practice, [1]. The following result by the Horodecki’s showing the existence of so-called entanglement witnesses is well known [11]:

**Theorem 3.** A mixed state $\sigma$ is separable iff $\text{Tr}(A\sigma) \geq 0$, for any bounded operator $A$ satisfying $\text{Tr}(A \cdot P \otimes Q) \geq 0$, for all product pure state $P \otimes Q$.

The above result was used by the Horodecki’s to show a bijection between entanglement witnesses and non-CP maps. This yields the following result which will be used to construct examples of separable states

**Theorem 4.** If a mixed state $\sigma \in L(\mathcal{H}_A) \otimes L(\mathcal{H}_B)$ is such that for every positive map $\Phi$ from $L(\mathcal{H}_B)$ to $L(\mathcal{H}_A)$, the operator $(I_A \otimes \Phi)(\sigma)$ is positive, then $\sigma$ is separable.

From the discussion above, we see that if one has a certainly family $S$ of states where any positive map restricted to $S$ is a completely positive map, then $\{S\}$ must consist of only separable states, due to lack of entanglement witnesses. We now obtain such families via the factorization of quadratic forms with matrix coefficients. Namely, we will apply the following result due to Calderon [3]:

**Theorem 5.** Let $F$ be a quadratic form $F(s, t) = \alpha_1 s^2 + \alpha_2 st + \alpha_3 t^2$ whose coefficients $\alpha_i$ lie in $C^{m \times m}$ and the indeterminates $s$ and $t$ are real. If $F$ is positive for all $s$ and $t$ then $F(s, t) = (\beta_1 s + \beta_2 t)^*(\beta_1 s + \beta_2 t)$, with $\beta_i \in C^{k \times m}$.

Choi applied the above result and obtained that if $\Phi : C^{2 \times 2} \rightarrow C^{m \times m}$ is positive, then there exists $V_i \in C^{2 \times m}$ s.t. $\Phi(A) = \sum_i V_i^* A V_i$ for all symmetric $A \in C^{2 \times 2}$. In other words, [5] effectively showed that:

**Proposition 1.** Let $S$ denote the set of $2 \times 2$ symmetric matrices. Any mixed state $\sigma \in C^{m \times m} \otimes S$ is separable

**Proof:** Let $\sigma$ be a mixed state of the form

$$
\sigma = \begin{bmatrix}
\sigma_{11} & \cdots & \sigma_{1m} \\
\vdots & \ddots & \vdots \\
\sigma_{m1} & \cdots & \sigma_{mm}
\end{bmatrix}
$$

, where each $\sigma_{ij}$ is $2 \times 2$ symmetric. For any positive map $\Phi : C^{2 \times 2} \rightarrow C^{m \times m}$, we have

$$
(I_m \otimes \Phi)(\sigma) = \sum_k \begin{bmatrix}
V_k^* \sigma_{11} V_k & \cdots & V_k^* \sigma_{1m} V_k \\
\vdots & \ddots & \vdots \\
V_k^* \sigma_{m1} V_k & \cdots & V_k^* \sigma_{mm} V_k
\end{bmatrix} = \sum_k (I \otimes V_k)^* \sigma (I \otimes V_k) \geq 0. \diamondsuit
$$
Remark 3. In particular, if a $2m \times 2m$ positive matrix is Hankel, when viewed as a scalar matrix, then it is separable as a $m \otimes 2$ state.

Using the SC parameters, this can be generalized to higher dimensions in a systematic way, although we will still be restricted to positive matrices that can be parametrized by two real parameters. To illustrate this, consider the following $3 \times 3$ case.

Proposition 2. Let $A \in C^{3 \times 3}$ be of the form

$$A = \begin{bmatrix} a & a & b \\ a & a & b \\ b & b & c \end{bmatrix}$$

For all positive $\Phi : C^{3 \times 3} \to C^{m \times m}$, where $m$ is arbitrary, there exists $V_i \in C^{3 \times m}$ s.t. $\Phi(A) = \sum_i V_i^* A V_i$.

Proof: By positivity of $\Phi$, we have

$$\Phi(\begin{bmatrix} s^2 & s^2 & st \\ s^2 & s^2 & st \\ st & st & t^2 \end{bmatrix}) \geq 0.$$ 

The positivity of the matrix in the argument of $\Phi$ can be directly checked using the SC parametrization. One can simply pick all the contractions in the SC parametrization of positive scalar matrices to be 1. This means the following quadratic form:

$$F(s, t) = s^2 \cdot \Phi(E_{11} + E_{12} + E_{21} + E_{22}) + st \cdot \Phi(E_{13} + E_{23} + E_{31} + E_{32}) + t^2 \cdot \Phi(E_{33}) \geq 0$$

for all real $s$ and $t$. By Calderon’s result, we have $\Phi(E_{11} + E_{12} + E_{21} + E_{22}) = C^*C$, $\Phi(E_{33}) = D^*D$, and $\Phi(E_{13} + E_{23} + E_{31} + E_{32}) = C^*D + D^*C$, where $C, D \in C^{k \times m}$ for some integer $k$. Let $\Phi' : C^{3 \times 3} \to C^{m \times m}$ be defined by its Choi matrix:

$$M_{\Phi'} = (\Phi'(E_{ij}))_{ij} = \begin{bmatrix} \frac{1}{4}C^*C & \frac{1}{4}C^*C & \frac{1}{4}C^*D \\ \frac{1}{4}C^*C & \frac{1}{4}C^*C & \frac{1}{4}C^*D \\ \frac{1}{4}D^*C & \frac{1}{4}D^*C & \frac{1}{2}D^*D \end{bmatrix}.$$ 

Again from the SC parametrization, the above matrix is manifestly positive. So $\Phi'$ is completely positive. If $A$ is of the specified form, then

$$\Phi(A) = a \cdot \Phi(E_{11} + E_{12} + E_{21} + E_{22}) + b \cdot \Phi(E_{13} + E_{23} + E_{31} + E_{32}) + c \cdot \Phi(E_{33})$$

$$= a \cdot C^*C + b \cdot (C^*D + D^*C) + c \cdot D^*D$$

$$= a \cdot \Phi'(E_{11} + E_{12} + E_{21} + E_{22}) + b \cdot \Phi'(E_{13} + E_{23} + E_{31} + E_{32}) + c \cdot \Phi'(E_{33})$$

$$= \Phi'(A).$$
Now take \( \{V_i\} \) to be any set of Kraus operators of \( \Phi' \) and this completes the proof. ♦

This translates to:

**Proposition 3.** Let \( S_1 \subset C^{3 \times 3} \) denote the family of matrices of the same form as \( A \) in the above proposition, then any mixed state \( \rho \in C^{m \times m} \otimes S_1 \), where \( m \) is arbitrary, is separable.

It is evident from the SC parameters that \( S_1 \) can be replaced by:

\[
S_2 = \{ A \in C^{3 \times 3} \mid A = \begin{bmatrix}
a & c & a \\
c & b & c \\
a & c & a
\end{bmatrix} \}
\]

or

\[
S_3 = \{ A \in C^{3 \times 3} \mid A = \begin{bmatrix}
a & c & c \\
c & b & b \\
c & b & b
\end{bmatrix} \}.
\]

The general procedure using the above approach is as follows. Let \( n \) be the size of each block. In the SC parametrization of positive scalar matrices, let all contractions be 1. Choose disjoint sets of indices \( I_s \) and \( I_t \) such that \( I_s \cup I_t = \{1, \ldots, n\} \). Denote the cardinality of \( I_s \) and \( I_t \) by \( n_s \) and \( n_t \) respectively. Consider the \( n \) diagonal elements from \( A = [a_{ij}] \in C^{n \times n} \). SC parametrize \( a_{ii} \) by \( s^2 \) if \( i \in I_s \) and \( a_{ii} \) by \( t^2 \) if \( i \in I_t \). For any positive map \( \Phi \), \( \Phi(A) \geq 0 \). Linearity of \( \Phi \) gives a positive quadratic form with coefficients in \( C^{n \times n} \):

\[
\Phi(A) = s^2(\sum_{i,j \in I_s} \Phi(E_{ij})) + st(\sum_{i \in I_s, j \in I_t} \Phi(E_{ij}) + \Phi(E_{ji})) + t^2(\sum_{i,j \in I_t} \Phi(E_{ij})) \geq 0
\]

for all \( s \) and \( t \). Calderon’s result gives

\[
\sum_{i,j \in I_s} \Phi(E_{ij}) = C^*C, \quad \sum_{i \in I_s, j \in I_t} \Phi(E_{ij}) + \Phi(E_{ji}) = (C^*D + D^*C), \quad \sum_{i,j \in I_t} \Phi(E_{ij}) = D^*D
\]

for some \( C \) and \( D \). Define a linear map \( \Psi \) by

\[
\Psi(E_{ij}) = \begin{cases} 
\frac{1}{n_s^2}C^*C, & \forall i, j \in I_s, \\
\frac{1}{n_t^2}D^*D, & \forall i, j \in I_t, \\
\frac{1}{n_sn_t}C^*D, & \forall i \in I_s, j \in I_t.
\end{cases}
\]

and
\[
\Psi(E_{ij}) = \frac{1}{n_s n_t} D^* C, \quad \forall i \in I_t, j \in I_s.
\]

Inspecting the Choi matrix of \(\Psi\), \(\Psi(E_{ij})\) shows that \(\Psi\) is CP. Let \(A'\) be obtained from \(A\) by replacing \(s^2, t^2, \) and \(st\) by arbitrary complex numbers \(a, b,\) and \(c\) respectively. Then

\[
\Phi(A') = a \left( \sum_{i,j \in I_s} \Phi(E_{ij}) \right) + c \left( \sum_{i \in I_s, i \in I_t} \Phi(E_{ij}) + \Phi(E_{ji}) \right) + b \left( \sum_{i,j \in I_t} \Phi(E_{ij}) \right)
\]

\[
= a \cdot C^* C + c \cdot ( C^* D + D^* C ) + b \cdot D^* D
\]

\[
= a \cdot n_s n_t \frac{1}{n_s} C^* C + c \cdot n_s n_t \left( \frac{1}{n_s} C^* D + \frac{1}{n_t} D^* C \right) + b \cdot n_t \frac{1}{n_t^2} D^* D
\]

\[
= a \left( \sum_{i,j \in I_s} \Psi(E_{ij}) \right) + c \left( \sum_{i \in I_s, i \in I_t} \Psi(E_{ij}) + \Psi(E_{ji}) \right) + b \left( \sum_{i,j \in I_t} \Psi(E_{ij}) \right)
\]

\[
= \Psi(A').
\]

Thus any positive map \(\Phi\) is CP when restricted to matrices of the form \(A'\) specified above. Let \(A'\) be the subspace of matrices of the form \(A'\), and \(S = A' \otimes C^{k \times k}\) for arbitrary \(k\). The correspondence between positive but non-CP maps and entanglement witnesses implies the result below.

**Theorem 6.** Any state \(\rho \in S\) is separable.

In this approach to obtain separable states, the SC parametrization was used twice: to get a subfamily of positive matrices that can be parametrized by two real parameters, and to ensure the proposed map \(\Psi\) has a positive Choi matrix, therefore CP. A natural question is whether this can be extended by varying the contractions in the parametrization of scalar positive matrices, i.e., by picking contractions which are not all equal to 1. To illustrate the issues at hand, consider a \(3 \times 3\) case. Suppose one parametrize a subfamily of \(3 \times 3\) positive matrices in the following way. Let

\[
A = \begin{bmatrix}
    s^2 & sat & s\beta s \\
    tat & t^2 & t\gamma s \\
    s\beta s & s\gamma t & s^2
\end{bmatrix} \geq 0
\]

where \(\alpha, \beta,\) and \(\gamma\) are specified by some chosen contractions \(\Gamma_i, i = 1, 2, 3,\) from the SC parameters. The proposed map \(\Psi\) would then have as its Choi matrix

\[
M_\Psi = \begin{bmatrix}
    \frac{1}{2+\beta+\beta} C^* C & \frac{\alpha}{\alpha+\gamma} C^* D & \frac{\beta}{\alpha+\gamma} C^* C \\
    \frac{\alpha}{\alpha+\gamma} D^* C & \frac{\alpha}{\alpha+\gamma} C^* D & \frac{\beta}{\alpha+\gamma} D^* C \\
    \frac{\beta}{\alpha+\gamma} C^* C & \frac{\beta}{\alpha+\gamma} D^* C & \frac{1}{2+\beta+\beta} C^* C
\end{bmatrix}
\]

where \(C\) and \(D\) are obtained the same way as before. To get \(M_\Psi \geq 0\), we apply the operator version of SC parametrization and find suitable contractions for the above
operator matrix. This amounts to solving a system of nonlinear inequations on unit disks. For instance, the $2 \times 2$ leading minor

$$\begin{bmatrix}
\frac{1}{2+\beta+\bar{\beta}} C^* C & \frac{\alpha}{\alpha+\bar{\gamma}} C^* D \\
\frac{\alpha}{\alpha+\bar{\gamma}} D^* C & D^* D
\end{bmatrix}$$

corresponds to the inequation

$$\left| \frac{1}{(2 + \beta + \bar{\beta})^{1/2}} \right| \geq \left| \frac{\alpha}{\alpha + \bar{\gamma}} \right|$$
in the variables $\Gamma_i, i = 1, 2, 3$. Determining the freedom in choosing $\Gamma_i$ amounts to solving the corresponding system of inequations.

Direct application of Schur parameters to obtain separable states: In the channel-state duality, between states in $\mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$ and channels $\Phi : \mathcal{L}(\mathcal{H}_A) \rightarrow \mathcal{L}(\mathcal{H}_B)$, any square-root factorization of the state gives a set of Kraus operators for the dual channel. In this duality the channel $\Phi$’s dual (unnormalized) state is precisely the Choi matrix $M_\Phi$. The following fact is easy to verify:

Let $\rho$ be a $n \times m$ bipartite mixed state. $\rho$ is separable iff its dual channel has a Kraus representation in which all non-zero Kraus operators have rank 1. The difficulty with applying this condition is that Kraus representations are not unique, and it is entirely conceivable that there are different Kraus representations some of which have this property, while the others do not. Hence, effectively this condition is typically only sufficient. Now, the SC parametrization explicitly calculates the Cholesky factors of positive matrices. The utility of this to the present context is that most of the Kraus operators produced by the Cholesky factorization tend to be sparse matrices (see [8] for the case of binary channels) and thus there is a greater chance of detecting a Kraus representation with all Kraus operators having rank one. We illustrate this via the case of $3 \otimes 3$ states.

Let a $3 \otimes 3$ state $\rho \in \mathbb{C}^{9 \times 9}$ have the Cholesky factorizations calculated from the Schur parameters $\rho = FF^*$, where $F = (F_{ij})_{1 \leq i,j \leq 9}$. By inspection, we see that the corresponding Kraus operators all have rank 1 if all of the following hold:

1. One of $D_{\Gamma_{i6}}, i = 1, \ldots, 5$ is 0, i.e. one of $|\Gamma_{i6}|, i = 1, \ldots, 5$, is 1.

2. One of $D_{\Gamma_{i5}}, i = 1, \ldots, 4$ is 0.

3. If $D_{\Gamma_{i6}} \neq 0$, for $i = 2, \ldots, 5$, then $D_{\Gamma_{i6}} = 0$ and $|\Gamma_{16}| = 1$, in which case we require $\Gamma_{15} = 0$.

3. We check via direct calculation if the Kraus operator corresponding to the fourth row of $F$ have rank 1.
4. \( D_{\Gamma_{23}} = 0 \) or \( D_{\Gamma_{13}} = 0 \).

5. \(|\Gamma_{12}| = 0\).

6. Finally, we check if the Kraus operator corresponding to the first row of \( F \) have rank 1.

As mentioned before, due to the non-uniqueness of Kraus representations, these are effectively only sufficient conditions. Indeed, if one were to apply a similar procedure to \( 2 \otimes 2 \) states, then there are block-Toeplitz matrices, which are known to satisfy the Peres-Horodecki PPT criterion (and would thus be separable), but which fail to satisfy the analogous set of conditions.

### 4. Jacobi Parametrization

While the SC parameters can be viewed as an extension of positive Toeplitz kernels, the Jacobi parameters generalize positive kernels of Hankel type, [9][10]. As with the SC case, we only give results relevant in the present context, together with informal derivations. A detailed presentation can be found in [9][10].

For a positive Hankel matrix

\[
H = \begin{bmatrix}
  s_0 & s_1 & s_2 & \cdots & s_n \\
  s_1 & s_2 & s_3 & \cdots & s_{n+1} \\
  \vdots & \vdots & \vdots & \ddots & \vdots \\
  s_n & s_{n+1} & \cdots & \cdots & s_{2n}
\end{bmatrix}
\]

Then it is known that there exists a symmetric tri-diagonal

\[
J = \begin{bmatrix}
  b_0 & a_1 & 0 & \cdots & 0 \\
  a_1 & b_1 & a_2 & \cdots & \vdots \\
  0 & a_2 & \ddots & \ddots & \vdots \\
  \vdots & \vdots & \ddots & \ddots & a_n \\
  0 & 0 & \cdots & a_n & b_n
\end{bmatrix}
\]

such that (notice by symmetry and Hermiticity \( a_i \)'s are real while \( b_i \)'s are complex)

\[ s_n = \langle J^n e_0, e_0 \rangle, \quad n > 0 \]

and

\[ s_0 = s_0 \langle e_0, e_0 \rangle \]
where $e_0 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$ is the basis element in $(n+1)$-dimensional Hilbert space. This yields the following Cholesky factorization of $H$:

$$H = \begin{bmatrix} \sqrt{s_0}e_0^* \\ (Je_0)^* \\ (J^2e_0)^* \\ \vdots \\ (J^ne_0)^* \end{bmatrix} \begin{bmatrix} \sqrt{s_0}e_0 & JJe_0 & J^2e_0 & \cdots & J^ne_0 \end{bmatrix}$$

Thus one might speculate that arbitrary positive matrices might have similar structures. Specifically, given an $(n+1) \times (n+1)$ positive matrix $(A_{ij})$, one may speculate that there may exist tri-diagonal $(n+1) \times (n+1)$ matrices $\{J_1, \cdots, J_n\}$ such that

$$A_{ij} = \langle J_i \cdots J_1e_0, J_j \cdots J_1e_0 \rangle.$$  

Such a parametrization is called a *tri-diagonal model* of positive matrices. A tri-diagonal would lead to the Cholesky factorization

$$A = \begin{bmatrix} s_0e_0^* \\ (J_1e_0)^* \\ (J_2J_1e_0)^* \\ \vdots \\ (J_n \cdots J_1e_0)^* \end{bmatrix} \begin{bmatrix} s_0e_0 & J_1e_0 & J_2J_1e_0 & \cdots & J_n \cdots J_1e_0 \end{bmatrix}$$

It was shown in [10] that there exists positive matrices which have no tridiagonal model. Instead, a general positive semi-definite can be described by what is called the *near tri-diagonal model*. Namely, the suitable matrices are given by

$$J_1 = \begin{bmatrix} b_0 & a_1 & 0 & 0 \\ a_1 & b_1 & a_2 & 0 \\ 0 & a_2 & b_2 & a_3 \\ 0 & 0 & a_3 & b_3 \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix},$$

$$J_2 = \begin{bmatrix} b_0 & e_{0,1} & 0 & 0 \\ a_1 & b_1 & a_2 & 0 \\ 0 & a_2 & b_2 & a_3 \\ 0 & 0 & a_3 & b_3 \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix},$$
The theorem below says any \((n+1) \times (n+1)\) positive semidefinite matrix can then be described by \(\{J_1, \cdots, J_n\}\) in the manner specified above. For the \(2 \times 2\) case, this is to say that any \(A = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} \geq 0\) can be written in the form

\[
A = \begin{bmatrix} s_0 & 0 \\ b_0 & a_1 \end{bmatrix} \begin{bmatrix} s_0 & b_0 \\ 0 & a_1 \end{bmatrix} = D_0^* D_1 = \begin{bmatrix} s_0^2 & s_0 b_0 \\ s_0 b_0 & |b_0|^2 + a_1^2 \end{bmatrix}
\]

for \(s_0 \geq 0\), which is obvious. To show a positive \(3 \times 3\)

\[
A = \begin{bmatrix} A_{00} & A_{01} & A_{02} \\ A_{10} & A_{11} & A_{12} \\ A_{20} & A_{21} & A_{22} \end{bmatrix}
\]

can be expressed via near tri-diagonal model, i.e.

\[
A = \begin{bmatrix} (s_0c_0)^* \\ (J_0^* c_0)^* \\ (J_1^* c_0)^* \end{bmatrix} \begin{bmatrix} s_0 c_0^* & J_0 c_0 & J_1 c_0 \end{bmatrix} = \begin{bmatrix} s_0 & 0 & 0 \\ b_0 & a_1 & 0 \\ \bar{b}_0^2 + \bar{c}_0 a_1 & a_1(b_0 + b_1) & a_1 a_2 \end{bmatrix} \begin{bmatrix} s_0 & b_0 & b_0^2 + c_0 a_1 \\ 0 & a_1 & a_1(b_0 + b_1) \\ 0 & 0 & a_1 a_2 \end{bmatrix} = \begin{bmatrix} D_0^* & 0 \\ \bar{b}_0^2 + \bar{c}_0 a_1 & a_1 \bar{b}_0 + b_1 & a_1 a_2 \\ 0 & a_1 a_2 \end{bmatrix} \begin{bmatrix} D_1 & 0 \\ 0 & \bar{a}_1^2 \end{bmatrix}
\]

The parameters \(s_0, b_0,\) and \(a_1\) can be assumed to be known from the \(2 \times 2\) case. Using the fact that there must exist a Cholesky factorization, there exist complex numbers \(x_1\) and \(x_2\) such that \(D_1 \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} A_{00} \\ A_{10} \end{bmatrix}\). Then \(c_{0,1}\) and \(b_1\) can be obtained by solving the equations \(x_1 = b_0^2 + c_{0,1} a_1\) and \(x_2 = a_1(b_0 + b_1)\) respectively. Using the usual argument for Cholesky factorizations one can calculate \(a_2 \geq 0\) easily.
Notice for the $3 \times 3$ case it is the parameter $c_{0,1}$ that allows the model to work. The general statement is:

**Theorem 7.** Given any $(n+1) \times (n+1)$ positive semidefinite matrix $A = (A_{ij})_{0 \leq i,j \leq n}$, there exists a near tri-diagonal model $\{J_1, \ldots, J_n\}$.

(Notice this statement is slightly different from that of [10] in that $A_{0,0}$ is not assumed to be 1 and positive definiteness is not required).

**Proof:** The proof uses exactly the same idea outline above. Assume the statement holds for the $n \times n$ case. We need to show

$$A = \begin{bmatrix} D_{n-1} & l_n \\ 0 & a_1 \cdots a_n \end{bmatrix}$$

where

$$l_n = J_n \cdots J_1 e_0$$

and $a_n \geq 0$ is to be determined. Again using the fact that there exists a Cholesky factorization, one can find $\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$ such that

$$D_{n-1} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} A_{0,n} \\ \vdots \\ A_{n-1,n} \end{bmatrix}.$$ 

The desired parameters can be obtained directly by solving the corresponding $n$ equations. ♦

As the combinatorial structure of SC parameters can be seen as given by the Dyck paths, the Jacobi parameters can be viewed via Lukasiewicz paths, [9 10].

5. **Jacobi Parameters and $2 \times 2$ Mixed States**

As mentioned in the introduction the Jacobi parametrization also produces the Cholesky factorization and yields a formula for the determinant analogous to the case for the SC parametrization. We will not repeat applications of these features similar to that in [3]. Instead, an elegant geometric picture for $2 \times 2$ states which is different from the so-called Bloch sphere emerges from the Jacobi parametrization.

A $2 \times 2$ positive semidefinite matrix $A$ can be Jacobi parametrized by

$$A = \begin{bmatrix} s_0 & 0 & 0 \\ b_0 & a_1 \\ 0 & s_0 b_0 \end{bmatrix} = D_1^* D_1 = \begin{bmatrix} s_0^2 & s_0 b_0 \\ s_0 b_0 & |b_0|^2 + a_1^2 \end{bmatrix}.$$
where \( s_0 \geq 0, a_1 \geq 0, \) and \( b_0 \) is complex. The trace 1 requirement means \( s_0^2 + a_1^2 + |b_0|^2 = 1. \) This essentially says that the \( 2 \times 2 \) mixed states lie in the following set in \( R^3: \)

\[
\{ s_0^2 + a_1^2 + \alpha^2 + \beta^2 = 1 | s_0 \geq 0, \ a_1 \geq 0 \}. 
\]

The pure states also have a nice description. We adopt the convention when \( s_0 = 0, b_0 = 1 \) (cf., the convention for the SC parameters in [8]). The general condition for the state to be pure is the state is pure iff \( a_1 = 0. \) This gives a set in \( R^3: \)

\[
S_1 = \{ s_0^2 + \alpha^2 + \beta^2 = 1 | s_0 \geq 0 \}
\]

which is exactly the surface of the upper hemisphere in \( R^3. \) When \( s_0 = 1 \) and \( |b_0| = 0, \) this is the classical \( |\text{up}\rangle \) state and it is at the pole of the hemisphere. When \( s_0 = 0 \) and \( b_0 = 1, \) this is the \( |\text{down}\rangle \) state and it is the point \((1, 0)\) in the \( xy\)-plane.

6. Conclusions

This brief note presented applications to the field of quantum information of two parametrizations of positive operator matrices, the SC and Jacobi parametrization, that Professor Tiberiu Constantinescu was instrumental in developing. These two applications are merely an indication of what is possible with these parametrizations. In our humble opinion these two parametrizations and the attendant characterizations of positive matrices are amongst the most versatile such characterizations. Related to these parametrizations are parametrizations of that other important class of matrices in quantum theory, viz., unitary matrices, which this note did not dwell upon. We hope that our presentation of these two parametrizations will stimulate readers into pursuing the various fascinating aspects (especially the combinatorial structures) of this subject in relation to quantum theory and its applications.

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