PARAMETRIZING QUANTUM STATES AND CHANNELS

T. CONSTANTINESCU AND V. RAMAKRISHNA

Abstract. This work describes one parametrization of quantum states and channels and several of its possible applications. This parametrization works in any dimension and there is an explicit algorithm which produces it. Included in the list of applications are a simple characterization of pure states, an explicit formula for one additive entropic quantity which does not require knowledge of eigenvalues, and an algorithm which finds one Kraus operator representation for a quantum operation without recourse to eigenvalue and eigenvector calculations.

1. Introduction

The interest in quantum information processing has brought added attention to questions of parametrizations of positive matrices. Indeed, at least two foundational ingredients in the theory of quantum information, viz., quantum states and quantum channels involve positive matrices. See, for instance, [16, 20]. Therefore it appears to be of interest to obtain descriptions (parametrizations) of the set of positive matrices.

The purpose of this note is to provide such an explicit parametrization by adapting similar results on positive definite kernels in [4]. This parametrization is rather intricate (and nonlinear), but in this paper we show some benefits of its use: the parameters of pure states are easily described; the parameters of a tensor product can be deduced from those of its factors; at least one entropic quantity (to be described in Section 3.3) is easy to compute; the Peres- Horodecki criterion for separability can be described explicitly described as inequalities for these parameters in low dimensions; purifications of qubits can be explicitly parametrized, and finally one Kraus operator representation for quantum operations can be computed without requiring any knowledge of the eigenvalues/eigenvectors of the associated Choi matrix.

The key features of this parametrization which are worth emphasizing are that it works in any dimension (indeed, it applies to matrices whose entries are operators themselves); there are explicit formulae for the parameters in terms of the entries of the matrix; while these are rather intricate, there is one computationally attractive algorithm which produces this parametrization; several quantities of interest can be computed via these parameters; the algorithm exploits the fact that the inherent structure in the matrix is inherited by its Schur complements and this results in the algorithm yielding (at least) one Cholesky decomposition of the matrix. Indeed, this last feature is precisely the reason why a Kraus operator representation of a quantum channel is produced by these parameters, without any need for eigenvalues or eigenvectors.
2. Preliminaries

In this section we introduce terminology and state the main result concerning the parametrization of positive (semidefinite) matrices.

2.1. Quantum states and channels. The state of a \( d \)-dimensional quantum system is described by a \( d \times d \) positive density matrix of trace 1, that is, a positive element of trace 1 in the algebra \( \mathcal{M}_d \) of complex \( d \times d \) matrices. States described by rank one density matrices are called pure states.

A quantum channel is a completely positive map \( \Phi : \mathcal{A} \rightarrow \mathcal{L}(\mathcal{H}) \) from a \( \mathcal{C}^* \)-algebra \( \mathcal{A} \) into the set \( \mathcal{L}(\mathcal{H}) = \mathcal{M}_d \), while \( \Phi \) is also required to be trace preserving. By the Stinespring theorem, [18], Theorem 4.1, such a map is the compression of a \( * \)-homomorphism. For \( \mathcal{A} = \mathcal{M}_d \), there is a somewhat more explicit representation, given in [2] (see also [9]). Thus, \( \Phi : \mathcal{M}_d \rightarrow \mathcal{L}(\mathcal{H}) \) is completely positive if and only if the matrix

\[
S_{\Phi} = [\Phi(E_{k,j})]_{k,j=1}^d
\]

is positive, where \( E_{k,j}, k, j = 1, \ldots, d \), are the standard matrix units of \( \mathcal{M}_d \). Each \( E_{k,j} \) is a \( d \times d \) matrix consisting of 1 in the \((k,j)\)th entry and zeros elsewhere. We notice that if \( X = [X_{k,j}]_{k,j=1}^d \), then \( Y = [Y_{k,j}]_{k,j=1}^d = \Phi(X) \) is given by the relations

\[
Y_{k,j} = \sum_{l,m} \Phi(E_{l,m})_{k,j} X_{l,m}.
\]

This shows that there is a one-to-one correspondence between the set of completely positive maps on \( \mathcal{M}_d \) with values in \( \mathcal{L}(\mathcal{H}) \) and the set of positive matrices in \( \mathcal{M}_d \otimes \mathcal{L}(\mathcal{H}) \).

For a linear map \( \Phi : \mathcal{M}_d \rightarrow \mathcal{M}_d \) the adjoint \( \hat{\Phi} \) is defined with respect to the Hilbert space structure on \( \mathcal{M}_d \) given by the Hilbert-Schmidt inner product \( \langle A, B \rangle = Tr(A^*B) \), where \( A^* \) denotes the adjoint of \( A \). It is easily seen that \( \hat{\Phi} \) is trace preserving if and only if \( \hat{\Phi} \) is unital (\( \hat{\Phi}(I) = I \)).

2.2. A parametrization of positive matrices. We describe a parametrization of the positive matrices in \( \mathcal{M}_d \otimes \mathcal{L}(\mathcal{H}) \), with \( \mathcal{H} \) allowed to be infinite-dimensional. Note that if \( \text{dim}(\mathcal{H}) = 1 \), such matrices are precisely \( d \times d \) positive matrices with complex entries. To that end, some elements of dilation theory ([18]) are needed. Let \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \) be two Hilbert spaces, not necessarily finite dimensional, and let \( \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2) \) denote the set of all bounded linear maps operators from \( \mathcal{H}_1 \) into \( \mathcal{H}_2 \). The operator \( T \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2) \) is
called a contraction if \( \|T\| \leq 1 \). The defect operator of \( T \) is \( D_T = (I - T^*T)^{1/2} \), where \( T^* \) denotes the adjoint operator, (as well as the complex conjugate in case \( T \) is just a complex number) and let \( D_T \) denote the closure of the range of \( D_T \). To any contraction \( T \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2) \) is associated the unitary operator \( U(T) : \mathcal{H}_1 \oplus D_T \to \mathcal{H}_2 \oplus D_T \) by the formula:

\[
U(T) = \begin{bmatrix} T & D_T^* \\ D_T & -T^* \end{bmatrix}.
\]

Now let \( \{\mathcal{F}_k\}_{k=1}^d \) be a family of Hilbert spaces and consider \( \{\Gamma_{k,j} \mid k, j = 1, \ldots, d, k \leq j\} \) a family of contractions such that (i) \( \Gamma_{k,k} = 0 \) for \( k = 1, \ldots, d \) and (ii) for \( k < j \),

\[
\Gamma_{k,j} \in \mathcal{L}(\mathcal{D}_{\Gamma_{k+1,j}}, \mathcal{D}_{\Gamma_{k,j-1}}).
\]

Unitary operators \( U_{k,j} \) are associated to this family by the recursions: \( U_{k,k} = I_{\mathcal{F}_k} \), the identity operator on \( \mathcal{F}_k \), \( k = 1, \ldots, d \), while for \( j > k \),

\[
U_{k,j} = U_{j-k}(\Gamma_{k,k+1})U_{j-k}(\Gamma_{k,k+2}) \ldots U_{j-k}(\Gamma_{k,j})U_{k+1,j} \oplus I_{\mathcal{D}_{\Gamma_{k,j}}},
\]

where \( U_{j-k}(\Gamma_{k,k+l}) \) denotes the unitary operator defined from the space

\[
(\oplus_{m=1}^{l-1} \mathcal{D}_{\Gamma_{k+1,m}}) \oplus (\mathcal{D}_{\Gamma_{k+1,l}} \oplus \mathcal{D}_{\Gamma_{k,l}}) \oplus (\oplus_{m=l+1}^{j} \mathcal{D}_{\Gamma_{k,m}})
\]

onto the space

\[
(\oplus_{m=1}^{l-1} \mathcal{D}_{\Gamma_{k+1,m}}) \oplus (\mathcal{D}_{\Gamma_{k+l-1}} \oplus \mathcal{D}_{\Gamma_{k,l}}) \oplus (\oplus_{m=l+1}^{j} \mathcal{D}_{\Gamma_{k,m}})
\]

by the formula

\[
U_{j-k}(\Gamma_{k,k+l}) = I \oplus U(\Gamma_{k,k+l}) \oplus I.
\]

The foregoing considerations from dilation theory will now be applied to matrices. Let \( S = [S_{k,j}]_{k,j=1}^d \) be a matrix such that \( S_{k,j} \in \mathcal{L}(\mathcal{H}) \) and let \( S_{k,k} = L_{k,k}^*L_{k,k} \) be a factorization of \( S_{k,k} \), \( k = 1, \ldots, d \). Denote the closure of the range of \( L_{k,k} \) by \( \mathcal{F}_k \), \( k = 1, \ldots, d \). For a family of contractions \( \Gamma_{k,j} \) as in the previous paragraph, denote by \( R_{k,j} \) the row contraction

\[
R_{k,j} = \begin{bmatrix} \Gamma_{k,k+1} & D_{\Gamma_{k,k+1}} \Gamma_{k,k+2} & \cdots & D_{\Gamma_{k,k+1}} \Gamma_{k,j-1} \\ \Gamma_{k,k+2} & \cdots & D_{\Gamma_{k,k+1}} \Gamma_{k,j-1} \\ \vdots & \ddots & \ddots & \vdots \\ \Gamma_{k,j-1} & \cdots & D_{\Gamma_{k,k+1}} \Gamma_{k,j-1} & \cdots \end{bmatrix}
\]

and by \( C_{k,j} \) the column contraction

\[
C_{k,j} = \begin{bmatrix} \Gamma_{j-1,j} & \cdots & \Gamma_{j-2,j} & \cdots & \Gamma_{k,j} D_{\Gamma_{k+1,j}} & \cdots & D_{\Gamma_{k+1,j}} \Gamma_{j-1,j} \end{bmatrix}^t,
\]

where "t" stands for matrix transpose. We now obtain the following characterization and structure of a positive matrix.

**Theorem 1.** The matrix \( S = [S_{k,j}]_{k,j=1}^d \) as above, satisfying \( S_{k,k}^* = S_{k,j} \), is positive if and only if i) \( S_{k,k} \geq 0, k = 1, \ldots, d \) and ii) there exists a family \( \{\Gamma_{k,j} \mid k, j = 1, \ldots, d, k \leq j\} \) of contractions such that \( \Gamma_{k,k} = 0 \) for \( k = 1, \ldots, d \) and Equation (2.4) is valid, and

\[
S_{k,j} = L_{k,k}^* (R_{k,j-1}U_{k+1,j-1}C_{k+1,j} + D_{\Gamma_{k+1}} \Gamma_{k+1,j} \Gamma_{j-1,j} L_{j,j} ).
\]
For a proof see Appendix 1. The $\Gamma_{kj}, j \neq k$ form the parametrization of positive matrices referred to in Section 1. Note the $\Gamma_{kk}$ are just some fake parameters, included in the statement of the theorem to avoid an artificial separation of the $j = k + 1$ case from that for other values of $j$. Note that when the dimension of $\mathcal{H} = 1$, these contractions, $\Gamma_{kj}$, are complex numbers in the closed unit disc.

Though this result looks rather intricate it provides a true parametrization of the set of positive matrices, has a useful physical interpretation, and does not depend on the dimension of $\mathcal{H}$. Furthermore, by adopting certain natural conventions, this can be even turned into a one-one parametrization of quantum states. One illustration of this is provided in Section 3, for the $d = 2$ case.

Let us next look at some concrete examples of Theorem 1. For $d = 2$ the result is well-known (see, e.g. [18]). For $d = 3$, the structure is more interesting, even in the scalar case $\dim \mathcal{H} = 1$. Thus, let

$$S = \begin{bmatrix} S_{11} & S_{12} & S_{13} \\ S_{12}^* & S_{22} & S_{23} \\ S_{13}^* & S_{23}^* & S_{33} \end{bmatrix}$$

be a positive matrix. Theorem 1 gives:

$$S_{12} = L_{12}^* \Gamma_{12} L_{22},$$
$$S_{23} = L_{23}^* \Gamma_{23} L_{33},$$
$$S_{13} = L_{13}^* \left( \Gamma_{12} \Gamma_{23} + D_{\Gamma_{12}}^{\Gamma_{23}} \Gamma_{13} \Gamma_{23} \right) L_{33},$$

and we can notice the connection between the structure of $S$ and spherical geometry in the formula for $S_{13}$. Thus, for $\Gamma_{12} = \cos \theta$, $\Gamma_{23} = \cos \theta_1$ and $\Gamma_{13} = \cos \phi$, the above formula for $S_{13}$ reduces to the cosine law in spherical geometry.

We also write the case $d = 4$ explicitly, with $\mathcal{H}$ of arbitrary dimension; in this case, if $S = [S_{k,j}]_{k,j=1}^{4}$, then

$$S_{k,k+1} = L_{k,k}^* \Gamma_{k,k+1} L_{k,k+1}, \quad k = 1, 2, 3,$$
$$S_{k,k+2} = L_{k,k}^* \left( \Gamma_{k,k+1} \Gamma_{k,k+2} + D_{\Gamma_{k,k+1}}^{\Gamma_{k,k+2}} \Gamma_{k,k+2} \Gamma_{k,k+2} \right) L_{k,k+2}, \quad k = 1, 2,$$

and

$$S_{14} = L_{11}^* \left( \Gamma_{12} \Gamma_{23} \Gamma_{34} + D_{\Gamma_{12}}^{\Gamma_{23}} \Gamma_{13} \Gamma_{23} \Gamma_{34} + \Gamma_{12} D_{\Gamma_{23}}^{\Gamma_{34}} \Gamma_{24} \Gamma_{34} \right) L_{44}.$$
where the upper-triangular operator $G_{1,d}$ is defined recursively by $G_{k,k} = I$, $k = 1, \ldots, d$, and for $1 \leq k < j \leq d$,

$$G_{k,j} = \begin{bmatrix} G_{k,j-1} & U_{k,j-1}C_{k,j} \\ 0 & D_{\Gamma_{k,j}} \cdots D_{\Gamma_{j-1,j}} \end{bmatrix}.$$  

These lattice structures can alternatively be described in the form of a time-varying, discrete transmission-line (string) For more details see [4], where this connection is described in the context of displacement structures. In the invariant time case, this transmission line is familiar in marine seismology, where the one-sided perfect reflector is given by the interface air-water, see [3]. The implications of this classical model for quantum states remain to be fully worked out. However, this model explains the intriguing fact that the number of summands in the formula for $S_{k,k+l}$, $l = 0, 1, \ldots$, in Theorem 1, is precisely the $l$th Catalan number. These observations will be explained elsewhere.

3. Parametrization of states

In this section we parametrize (finite dimensional) quantum states by using Theorem 1 and we show several applications of this parametrization. Throughout this section, except in Subsection 3.2, we will write the $\Gamma_{k,l}$ and the $D_{\Gamma_{k,l}}$ of the previous section as $g_{k,l}$ and $d_{k,l}$ respectively, so as to distinguish states from channels. The explicit formulae for the parameters, $g_{k,l}$, depend on the basis of $\mathcal{M}_d$ and it is often convenient to use selfadjoint bases containing the identity (see, for instance, [26], [12]). Such an orthogonal basis can be obtained from $\{E_{k,j}\}_{k,j=1}^d$ as follows:

$$f_{k,j}^d = E_{k,j} + E_{j,k}, \quad k < j,$$

$$f_{k,j}^d = \frac{1}{i} (E_{j,k} - E_{k,j}), \quad k > j,$$

$$h_1^d = I_d, \quad h_k^d = h_k^{d-1} \oplus 0, \quad 1 < k < d, \quad h_d^d = \sqrt{\frac{2}{d(d-1)}} \left( h_1^{d-1} \oplus (1-d) \right).$$

For $d = 2$, we deduce

$$h_1^2 = I_2, f_{12}^2 = \sigma_1, f_{21}^2 = \sigma_2, h_2^2 = \sigma_3,$$

where $\sigma_1$, $\sigma_2$, $\sigma_3$ are the Pauli matrices. In the Pauli basis a hermitian matrix with trace 1 will be represented as $\rho = \frac{1}{2}(I_2 + \sum_{k=1}^3 \beta_k \sigma_k)$ and its positivity is equivalent to the Bloch sphere condition $1 - \|\beta\|^2 \geq 0$. By using Theorem 1 the positivity of $\rho$ is equivalent to a cylinder condition on the parameter $(\beta_3, g)$:

$$|\beta_3| \leq 1,$$

$$\beta_1 - i\beta_2 = (1 - |\beta_3|^2)^{1/2} g, \quad |g| \leq 1,$$

and in order to ensure a one-to-one parametrization we choose $g = 0$ if $|\beta_3| = 1$. 

For \( d = 3 \) we obtain the Gell-Mann matrices:

\[
h_1^3 = I_3, \quad h_2^3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad h_3^3 = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix}, \ldots
\]

A hermitian matrix of trace 1 will be represented as

\[
\rho = \frac{1}{3} \left( I_3 + \beta_2 h_2^3 + \beta_3 h_3^3 + \sum_{k \neq j} \gamma_{k,j} f_{k,j}^3 \right).
\]

By using Theorem \( \text{I} \) the positivity of \( \rho \) is equivalent to the conditions:

\[
1 + \beta_2 + \frac{\beta_3}{\sqrt{3}} \geq 0, \quad 1 - \beta_2 + \frac{\beta_3}{\sqrt{3}} \geq 0, \quad 1 - \frac{2\beta_3}{\sqrt{3}} \geq 0,
\]

\[
\gamma_{12} - i \gamma_{21} = ((1 + \frac{\beta_3}{\sqrt{3}})^2 - \frac{\beta_2^2}{3})^{1/2} g_{12}, \quad |g_{12}| \leq 1,
\]

\[
\gamma_{23} - i \gamma_{32} = (1 - \beta_2 + \frac{\beta_3}{\sqrt{3}})^{1/2}(1 - \frac{2\beta_3}{\sqrt{3}})^{1/2} g_{23}, \quad |g_{23}| \leq 1,
\]

\[
\gamma_{13} - i \gamma_{31} = (1 - \beta_2 + \frac{\beta_3}{\sqrt{3}})^{1/2}(1 - \frac{2\beta_3}{\sqrt{3}})^{1/2} (g_{12} g_{23} + (1 - |g_{12}|^2)^{1/2}(1 - |g_{23}|^2)^{1/2} g_{13}), \quad |g_{13}| \leq 1.
\]

The case \( d = 4 \) was explicitly written in \( \text{[5]} \), but with respect to the basis \( \sigma_k \otimes \sigma_j \). In any dimension we can write

\[
\rho = \frac{1}{n} \left( I_n + \sum_{l=2}^d \beta_l h_l^d + \sum_{k \neq j} \gamma_{k,j} f_{k,j}^d \right),
\]

and the parameters \( \beta_l \) appearing on the diagonal of \( \rho \) satisfy a system of linear inequalities, while the parameters \( g_{k,j} \) associated to the off-diagonal elements by Theorem \( \text{I} \) are almost independent: they belong to the closed unit disk and satisfy the boundary conditions (2.4).

3.1. Pure states. It was already noticed in \( \text{[5]} \) that the purity of qubits can be explicitly checked via the parameters of Theorem \( \text{I} \). Here we extend this result to any dimension. Let \( \rho \) be a \( d \)-dimensional state,

\[
\rho = \frac{1}{n} \left( I_n + \sum_{l=2}^d \beta_l h_l^d + \sum_{k \neq j} \gamma_{k,j} f_{k,j}^d \right) = \frac{1}{n} \sum_{k,j} \rho_{k,j} E_{k,j}.
\]

We notice that

\[
\rho_{k,k} = 1 + \sum_{l=2}^d \beta_l (h_l^d)_{k,k}, \quad k = 1, \ldots, d,
\]

and

\[
\rho_{k,j} = \gamma_{k,j} - i \gamma_{j,k}, \quad k < j.
\]

Let \( \{g_{k,j}\} \) be the parameters associated to the positive matrix \( \rho = [\rho_{k,j}]_{k,j=1}^d \) by Theorem \( \text{I} \).
Theorem 2. A state $\rho$ is pure if and only if the parameters $g_{k,j}$ are zero except for those indices for which $\rho_{k,k}\rho_{j,j} \neq 0$, in which case $|g_{k,j}| = 1$.

Proof. Assume $\rho$ is pure. This implies that each matrix
\[
\begin{bmatrix}
\rho_{k,k} & \rho_{k,k+1} \\
\rho_{k+1,k} & \rho_{k+1,k+1}
\end{bmatrix}
\]
has rank at most 1. This happens in case either at least one of $\rho_{k,k}$, $\rho_{k,k+1}$ is zero or if $|g_{k,k+1}| = 1$. It remains to see what happens if $\rho_{k,k} \neq 0$, $\rho_{k,l} = 0$ for $k < l < m$ and $\rho_{m,m} \neq 0$. In this situation we must have $\rho_{p,l} = 0$ for $k < p < l < m$, therefore $g_{p,l} = 0$ for $k < p < l < m$, and so, $\rho_{k,m} = \rho_{k,k}^{1/2}\rho_{m,m}^{1/2}$ by (2.5). Then, the fact that
\[
\begin{bmatrix}
\rho_{k,k} & \rho_{k,m} \\
\rho_{k,m}^* & \rho_{m,m}
\end{bmatrix}
\]
has rank at most 1 implies $|g_{k,m}| = 1$.

Conversely, we deduce from (2.5) that $\rho = \frac{1}{n}v_{\rho}v_{\rho}^*$, where the vector $v_\rho$ is described as follows: let $i_1 < \ldots < i_k$ be the indices of the nonzero diagonal elements of $\rho$. Then,
\[
(v_\rho)_{i_1} = \rho_{i_1,i_1}^{1/2},
\]
\[
(v_\rho)_{i_2} = \rho_{i_2,i_2}^{1/2}g_{i_1,i_2}^*,
\]
\[
\vdots
\]
\[
(v_\rho)_{i_k} = \rho_{i_k,i_k}^{1/2}g_{i_1,i_2}^* \cdots g_{i_{k-1},i_k}^*,
\]
while the other entries of $v_\rho$ are zero. $\square$

Thus, the vector in $C^d$ representing the pure state can also be written down in terms of the parameters. It was noticed in [5] that these parameters can be used in producing a one-one parametrization of purifications of qubits.

3.2. Tensor products. We next discuss producing parameters for tensor products of positive matrices, in terms of the parameters of the factors entering the product.

Let us begin with a very simple example. Take $S_1 = \begin{bmatrix} 1 & A_{12} \\ A_{12}^* & 1 \end{bmatrix}$ and $S_2 = \begin{bmatrix} 1 & B_{12} \\ B_{12}^* & 1 \end{bmatrix}$. Then
\[
S_1 \otimes S_2 = \begin{bmatrix}
1 & B_{12} & A_{12} & A_{12}B_{12} \\
B_{12}^* & 1 & A_{12}B_{12}^* & A_{12} \\
A_{12}^* & B_{12}A_{12} & 1 & B_{12} \\
B_{12}^*A_{12} & A_{12}^* & B_{12}^* & 1
\end{bmatrix}
\]
(note that we use the so-called right Kronecker product representation of the tensor product, see [1]). Formula (2.5) gives:
\[
\Gamma_{12} = B_{12}, \quad \Gamma_{23} = A_{12}B_{12}^*, \quad \Gamma_{34} = B_{12},
\]
\[
\Gamma_{13} = \frac{A_{12}(1 - |B_{12}|^2)^{1/2}}{(1 - |A_{12}|^2|B_{12}|^2)^{1/2}},
\]
\[
\Gamma_{24} = \frac{A_{12}(1 - |B_{12}|^2)^{1/2}}{(1 - |A_{12}|^2|B_{12}|^2)^{1/2}},
\]
\[
\Gamma_{14} = -A_{12}B_{12}.
\]

The fact that \(\Gamma_{14}\) has a simpler structure than expected indicates that there is additional structure that can be explored fruitfully. It turns out that in this case it is more convenient to search for a block lattice structure first.

Let \(S_1 = [S_{1,k,j}]_{k,j=1}^d\), \(S_2 = [S_{2,k,j}]_{k,j=1}^{d'}\) be two positive matrices. Also let \(\{\Gamma_{1,k,j}\}, \{\Gamma_{2,k,j}\}\) be the corresponding parameters associated by Theorem 1 to \(S_1\), respectively, \(S_2\). For a matrix \(T\) we use the notation \(T \oplus_p = T \oplus \ldots \oplus T\), to denote its \(p\)-fold direct sum.

**Theorem 3.** The positive matrix \(S_1 \otimes S_2\) is a \(d \times d\) block matrix with structure given by (2.5) with:

\[
L_{k,k} = G_{1,d'}^2(S_{1,k,k})^\oplus d', \quad k = 1, \ldots, d,
\]
\[
\Gamma_{k,j} = (\Gamma_{1,k,j})^\oplus d', \quad 1 \leq k < j \leq d,
\]

where \(G_{1,d'}^2\) is the upper triangular Cholesky factor of \(S_2\).

**Proof.** First, it is easily checked that

\[
S_1 \otimes S_2 = (G_{1,d'}^2)^\oplus d' \left[(S_{1,k,j})^\oplus d' \right]_{k,j=1}^d (G_{1,d'}^2)^\oplus d
\]

and then, some algebra with formula (2.5) gives that the parameters associated by Theorem 1 to the positive matrix \(\left[(S_{1,k,j})^\oplus d' \right]_{k,j=1}^d\) are \(\Gamma_{ij} = (\gamma_{ij}^1)^\oplus M\). □

It is quite convenient to use the Cholesky factor of \(S_2\) since it can be explicitly computed in terms of the parameters \(\Gamma_{2,k,j}\), as shown by (2.6).

3.3. Entropy. In this section we consider an entropy-like number \(E(\rho)\) that can be explicitly computed in terms of the parameters \(\{g_{k,j}\}\) of a state \(\rho\). This quantity, \(E(\rho) = \frac{1}{d} \text{Tr}(\log \rho)\), is mentioned in [17], as one of a list of candidates for a quantum notion of entropy. Further material about quantum entropies is summarized in [17].

One simple way to motivate \(E(\rho)\) is to start with the classical Kulback-Leibler information number,

\[
D(f\|g) = \int f(x)\log(f(x)/g(x))dx,
\]

where \(f\) and \(g\) are probability densities and \(x = (x_1, \ldots, x_n)\). If \(f\) and \(g\) are Gaussian with covariance matrices \(P\), respectively, \(R\), then

\[
D(f\|g) = -\frac{1}{2} \left( \log \det PR^{-1} + \text{tr}(I - PR^{-1}) \right).
\]
By setting, for instance \( R = \frac{1}{d}, \) we see that \(-E(\rho)\) is upto a constant \( D(f\|g)\). Thus, loosely speaking, in this view the classical analogue of a state is a Gaussian whose covariance matrix the density matrix is. The foregoing suggests the consideration of the following entropy of a \( d\)-dimensional state,

\[
E(\rho) = \frac{1}{d} \log \det(\rho) = \frac{1}{d} \sum_{k=1}^{d} \log \lambda_k,
\]

where \( \{\lambda_k\}_{k=1}^{d} \) is the set of eigenvalues of \( \rho \). This is a well-known formula giving a functional of entropy type (see [17]), and also plays a significant role in convex optimization, [15].

\( E \) behaves quite differently from the von Neumann entropy, for instance, pure states have vanishing von Neumann entropy while \( E(\rho) = -\infty \) for a pure state \( \rho \) (however, see below for one variation on \( E(\rho) \) which remedies this). Still, \( E \) has some interesting properties, two of them described by the following result.

**Theorem 4.** (a) Let \( \rho \) be a state with parameters \( \{g_{k,j}\} \). Then

\[
E(\rho) = \frac{1}{d} \left( \sum_{k=1}^{d} \log \rho_{k,k} + \sum_{k<j} \log(1 - |g_{kj}|^2) \right).
\]

(b) Let \( \rho \) and \( \psi \) be two states. Then

\[
E(\rho \otimes \psi) = E(\rho) + E(\psi).
\]

**Proof.** (a) Using Algorithm 10 and Th 11 yields (cf., Th 1.5.10 in [4])

\[
\det \rho = \left( \prod_{k=1}^{d} \rho_{k,k} \right) \prod_{k<j} (1 - |g_{kj}|^2).
\]

Taking the logarithm in this formula we obtain (3.1).

(b) This follows easily from the formula for the determinant of a tensor product of matrices. \( \square \)

We also notice that \( E(\rho) \leq \log d \), with equality for \( \rho_{11} = \ldots = \rho_{dd} = \frac{1}{d} \), which implies the following maximum entropy principle: if \( \rho \) is a given state, then for any dimension \( d' \) there is a state \( \psi_0 \) of dimension \( d' \) such that

\[
\max_{\psi} E(\rho \otimes \psi) = E(\psi_0),
\]

where the maximum is taken over all states \( \psi \) of dimension \( d' \).

One small variation on \( E \) is provided by the formula:

\[
E_0(\rho) = \frac{1}{d} \sum_{j=1}^{l} \log \lambda_{kj},
\]
where $\lambda_{kj} \in \mathbb{C}$, $j = 1, \ldots, l$, are the nonzero eigenvalues of $\rho$. We see that $E_0$ is still additive and $\rho$ is pure if and only if $E_0(\rho) = 0$. However, to apply (3.4), one must first find the restriction of $\rho$ to its support.

The key utility of using the parameters $g_{kj}$ is that there is no need for any eigenvalue computations for finding $E(\rho)$. Contrary to the situation with eigenvalues, the $g_{kj}$ can be related to the entries of $\rho$ via explicit formulae. 

3.4. The Peres-Horodecki Criterion. The parameters $\{g_{kj}\}$ of a state $\rho$ can be also used to explicitly write the finite set of inequalities characterizing the separability of $2 \times 2$ and $2 \times 3$ states. For $2 \times 2$ states we have the following result.

**Theorem 5.** Let $\rho$ be a $2 \times 2$ state with parameters $\{g_{kj}\}$. Then $\rho$ is separable if and only if:

$$
\rho_{12}^{1/2} \rho_{33}^{1/2} + \rho_{11}^{1/2} \rho_{44}^{1/2} d_{12} d_{13} d_{24} d_{34} \geq 0
$$

and the system of inequalities

$$
\begin{align*}
d_{12} (d_{23} + (1 - |h_{14}^2|)^{1/2}) &\geq |g_{12} g_{23} - \overline{g}_{12} \overline{g}_{23}|, \\
d_{34} (d_{23} + (1 - |h_{14}^2|)^{1/2}) &\geq |g_{34} g_{23} - \overline{g}_{34} \overline{g}_{23}|,
\end{align*}
$$

$$
\rho_{12}^{1/2} \rho_{33}^{1/2} + \rho_{11}^{1/2} \rho_{44}^{1/2} d_{12} (1 - |h_{14}^2|)^{1/2} (1 - |h_{24}^2|)^{1/2} d_{34} \geq 0
$$

admits solutions $h_{14}, h_{13}, h_{24}$ in the closed unit disk, subject to the boundary condition (2.4), where $d_{k,j} = (1 - |g_{kj}|^2)^{1/2}$.

**Proof.** The result is a consequence of the Peres-Horodecki characterization of $2 \times 2$ separable states, [8, 19], and Theorem 1. \hfill \Box

Similar inequalities can be written for $2 \times 3$ separable states.

4. Quantum Channels

In this section we analyse some consequences of Theorem 1 for the structure of quantum channels. We can immediately exemplify the case of binary channels.

**Example 6.** A detailed analysis of quantum binary channels is given in [22]. We show here how Theorem 1 relates to that analysis. It is showed in [13] that any quantum binary channel $\Phi$ has a representation

$$
\Phi(A) = U[\Phi_{t,A}(VAV^*)]U^*,
$$

where $U, V \in U(2)$ and $\Phi_{t,A}$ has the matrix representation

$$
T = \begin{bmatrix}
1 & 0 & 0 & 0 \\
t_1 & \lambda_1 & 0 & 0 \\
t_2 & 0 & \lambda_2 & 0 \\
t_3 & 0 & 0 & \lambda_3 \\
10
\end{bmatrix}
$$
with respect to the Pauli basis \( \{ I, \sigma_1, \sigma_2, \sigma_3 \} \) of \( \mathcal{M}_2 \). See [27] also for similar normal forms. We can obtain (formula (26) in [22]) that

\[
S_{\Phi t, A} = \frac{1}{2} \begin{bmatrix}
1 + t_3 + \lambda_3 & t_1 - it_2 & 0 & \lambda_1 + \lambda_2 \\
t_1 + it_2 & 1 - t_3 - \lambda_3 & \lambda_1 - \lambda_2 & 0 \\
0 & \lambda_1 - \lambda_2 & 1 + t_3 - \lambda_3 & t_1 - it_2 \\
\lambda_1 + \lambda_2 & 0 & t_1 + it_2 & 1 - t_3 + \lambda_3
\end{bmatrix}.
\]

Similarly, by formula (27) in [22],

\[
S_{\Phi t, A} = \frac{1}{2} \begin{bmatrix}
1 + t_3 + \lambda_3 & 0 & t_1 + it_2 & \lambda_1 + \lambda_2 \\
0 & 1 + t_3 - \lambda_3 & \lambda_1 - \lambda_2 & t_1 + it_2 \\
t_1 - it_2 & \lambda_1 - \lambda_2 & 1 - t_3 - \lambda_3 & 0 \\
\lambda_1 + \lambda_2 & t_1 + it_2 & 0 & 1 - t_3 + \lambda_3
\end{bmatrix}.
\]

It is slightly more convenient to deal with \( S = [S_{k,j}]_{k,j=1}^4 = 2S_{\Phi t, A} \). Formula [25] gives:

\[
S_{11} = 1 + t_3 + \lambda_3; \quad S_{22} = 1 + t_3 - \lambda_3; \quad S_{33} = 1 - t_3 - \lambda_3; \quad S_{44} = 1 - t_3 + \lambda_3;
\]

\[
\Gamma_{12} = 0, \quad \Gamma_{34} = 0;
\]

\[
S_{23} = S_{22}^{1/2} \Gamma_{23} S_{33}^{1/2},
\]

so that

\[
\Gamma_{23} = \frac{\lambda_1 - \lambda_2}{(1 + t_3 - \lambda_3)^{1/2}(1 - t_3 - \lambda_3)^{1/2}};
\]

\[
S_{13} = S_{11}^{1/2} \Gamma_{13} D_{\Gamma_{23}} S_{33}^{1/2},
\]

so that

\[
\Gamma_{13} = \frac{(t_1 + it_2)(1 + t_3 - \lambda_3)^{1/2}}{((1 + t_3 - \lambda_3)(1 - t_3 - \lambda_3) - (\lambda_1 - \lambda_2)^2)^{1/2}(1 + t_3 + \lambda_3)^{1/2}};
\]

\[
S_{24} = S_{22}^{1/2} D_{\Gamma_{23}} \Gamma_{24} S_{44}^{1/2},
\]

so that

\[
\Gamma_{24} = \frac{(t_1 + it_2)(1 - t_3 - \lambda_3)^{1/2}}{((1 + t_3 - \lambda_3)(1 - t_3 - \lambda_3) - (\lambda_1 - \lambda_2)^2)^{1/2}(1 - t_3 + \lambda_3)^{1/2}}.
\]

Finally,

\[
S_{14} = S_{11}^{1/2} (\Gamma_{13} \Gamma_{24}^* + D_{\Gamma_{23}} D_{\Gamma_{24}}) S_{44}^{1/2}.
\]

For brevity, we omit writing out the formula for \( \Gamma_{14} \). We deduce that \( \Phi_{t, A} \) is completely positive if and only if the following eight inequalities hold:

\[
S_{k,k} \geq 0, \quad k = 1, \ldots, 4,
\]

\[
|\Gamma_{23}| \leq 1, \quad |\Gamma_{13}| \leq 1, \quad |\Gamma_{24}| \leq 1, \quad |\Gamma_{14}| \leq 1.
\]

Further, we know what happens in the degenerate cases (i.e., the cases where any of these inequalities become equalities). Thus, the implication of \( S_{kk} = 0 \) for some \( k \) on the structure of \( \Phi_{t, A} \) is clear. Also, if \( |\Gamma_{23}| = 1 \), then necessarily \( t_1 = t_2 = 0 \) and
\[ \lambda_1 + \lambda_2 = (1 + t_3 + \lambda_3)^{1/2} \Gamma_{14}(1 - t_3 + \lambda_3)^{1/2} \text{ for some contraction } \Gamma_{14}. \]

If either \( |\Gamma_{13}| = 1 \) or \( |\Gamma_{24}| = 1 \), then necessarily \( \Gamma_{14} = 0 \) and \( S_{14} = S_{11}^{1/2}(-\Gamma_{13}^{*} \Gamma_{23} \Gamma_{24}) S_{14}^{1/2} \).

We notice that this result is of about the same nature as that in [22]. This is because the first step of (2.5), specialized to \( 4 \times 4 \) matrices (viz., the \( j = k+1 \) step), is precisely Lemma 6 in [22] which is used for the analysis in [22]. If we had instead used the block version of (2.5), i.e., viewing \( S_{\Phi} \) as a \( 2 \times 2 \) matrix with entries themselves \( 2 \times 2 \) matrices, then we would deduce precisely Theorem 1 of [22]. What we basically have done here is that we used (2.5) in order to deduce in a systematic way the condition that \( R_{\Phi, \Lambda} \) in Theorem 1 of [22] is a contraction. One advantage of doing this is that it works in higher dimensions.

It is noted that the correspondence between \( S_{\Phi} \) and the parameters \( \Gamma_{k,j} \) is nonlinear. Only for the first step is the correspondence affine and therefore can be used in the analysis of extreme points in the case \( d = 2 \), as it was done in [22]. This seems to be unclear for \( d > 2 \), at this moment.

4.1. Capacity. It is worth remarking that the suggested notion of quantum entropy from Section (3.3) could be used to posit a notion of channel capacity for quantum channels, which is trivially additive. Several numbers have been suggested to define the capacity of a quantum channel, with additivity as a desirable requirement. See, for instance, [23, 25]. While additivity of some these notions has been demonstrated for special classes of channels, such as entanglement breaking channels, conjectures in the direction of additivity for some other notions were recently disproved (25). Therefore, it might be useful to have some other possible candidates. Motivated by the discussion in Section 3.3 we introduce for a quantum channel \( \Phi : \mathcal{M}_d \rightarrow \mathcal{M}_d' \) the number

\[
D(\Phi) = -\frac{1}{N} \log \det S_{\Phi},
\]

where \( N = dd' \). Trivially, \( D(\Phi) \) is additive, and there is an explicit expression for it in terms of the parameters \( \Gamma_{k,j} \) of \( S_{\Phi} \):

\[
D(\Phi) = -\frac{1}{N} \left( \sum_{k=1}^{N} \log S_{k,k} + \sum_{k<j} \log(1 - |\Gamma_{k,j}|^2) \right).
\]

Once again, \( D(\Phi) \geq \log n \) and a minimum capacity principle holds: given \( \Phi \), there exists a quantum channel \( \Psi \) such that

\[
\min_{\Psi} D(\Phi \otimes \Psi)
\]

is attained. As an example of explicit computation of \( D(\Phi) \), we consider binary quantum channels as in Example 6. For simplicity, assume \( t_1 = t_2 = t_3 = 0 \). Then, using the parameters calculated in Example 6 we deduce

\[
D(\Phi) = -1/4 \left( 2 \log \left( \frac{1+\lambda_2}{2} \right) + 2 \log \left( \frac{1-\lambda_2}{2} \right) + \log \left( 1 - \left| \frac{\lambda_1 - \lambda_2}{1+\lambda_3} \right|^2 \right) + \log \left( 1 - \left| \frac{\lambda_1 + \lambda_2}{1+\lambda_3} \right|^2 \right) \right).
\]
4.2. Connections with Kraus representations. In this subsection, we provide one explicit Kraus operator representation for any channel, which does not require either eigenvalues or eigenvectors of the associated Choi matrix. While Kraus representations are not unique, they are very useful in explicit computations involving quantum channels. For instance, one can write down at least one Stinespring dilation in terms of a Kraus representation, and thus at least one mock unitary operation for a quantum channel; a formula for entanglement fidelity of a channel can be computed in terms of them; sufficient conditions for either unitarity or the entanglement breaking property can be checked; they play a role in quantum error correcting codes, quantum tomography etc., See, for instance, [16, 20, 7].

Consider a quantum channel \( \Phi : \mathcal{M}_d \to \mathcal{M}_d \). A familiar representation of quantum channels is the Kraus representation, [14],

\[
\Phi(\rho) = \sum_{k=1}^{d^2} A_k^* \rho A_k,
\]

where \( A_k \in \mathcal{M}_d \), \( k = 1, \ldots, d^2 \), are called the generators of \( \Phi \), and \( \sum_{k=1}^{d^2} A_k A_k^* = I \).

The connection between the Kraus representation and \( S_\Phi \) is given by the formula

\[
(4.2) \quad S_\Phi = A^* A,
\]

where

\[
A = \begin{bmatrix}
\text{row}(A_1) \\
\vdots \\
\text{row}(A_{d^2})
\end{bmatrix}
\]

and

\[
\text{row}(A_k) = \begin{bmatrix}
(A_k)_{11} & \cdots & (A_k)_{1d} & (A_k)_{2d} & \cdots & (A_k)_{2d} & \cdots & (A_k)_{d1} & \cdots & (A_k)_{dd}
\end{bmatrix}.
\]

This relation shows that while the generators of a Kraus representation are not unique, they will give the same channel provided that (4.2) holds. In particular, we can choose Kraus generators using the Cholesky factorization of \( S_\Phi \). As mentioned before, the algorithms for finding the parameters, \( \Gamma_{kj} \), systematically yield a Cholesky factorization of a positive matrix. We give the details for binary channels.

**Example 7.** Let \( S_\Phi : \mathcal{M}_2 \to \mathcal{M}_2 \) be a binary channel and let \( \{\Gamma_{k,j}\} \) be the parameters of \( \Phi \) given by Theorem II. Using formula (2.6), we deduce

\[
G_{14} = \begin{bmatrix}
L_{11} & \Gamma_{12} L_{22} & Z L_{33} & W L_{44} \\
0 & D_{\Gamma_{12}} L_{22} & (D_{\Gamma_{12}} \Gamma_{23} - \Gamma_{12}^* \Gamma_{13} D_{\Gamma_{23}}) L_{33} & X L_{44} \\
0 & 0 & D_{\Gamma_{13}} D_{\Gamma_{23}} L_{33} & Y L_{44} \\
0 & 0 & 0 & D_{\Gamma_{14}} D_{\Gamma_{24}} D_{\Gamma_{34}} L_{44}
\end{bmatrix},
\]

with

\[
X = D_{\Gamma_{12}} \Gamma_{23} \Gamma_{34} + D_{\Gamma_{12}} D_{\Gamma_{23}}^* \Gamma_{24} D_{\Gamma_{34}} - \Gamma_{12}^* D_{\Gamma_{13}} \Gamma_{14} D_{\Gamma_{24}} D_{\Gamma_{34}},
\]

and

\[
Y = D_{\Gamma_{13}} D_{\Gamma_{24}} \Gamma_{34} + D_{\Gamma_{13}} D_{\Gamma_{23}} \Gamma_{24} D_{\Gamma_{34}} - \Gamma_{13} \Gamma_{14} D_{\Gamma_{24}} D_{\Gamma_{34}}.
\]
\[ Y = D_{\Gamma_{13}} D_{\Gamma_{23}} \Gamma_{34} - D_{\Gamma_{13}}^* \Gamma_{23}^* D_{\Gamma_{24}} D_{\Gamma_{34}}, \]
\[ Z = \Gamma_{12} \Gamma_{23} + D_{\Gamma_{12}}^* D_{\Gamma_{23}}, \]
and
\[ W = \Gamma_{12} \Gamma_{23} \Gamma_{34} + D_{\Gamma_{12}}^* \Gamma_{13} D_{\Gamma_{23}} \Gamma_{34} + \Gamma_{12} D_{\Gamma_{23}} \Gamma_{24} D_{\Gamma_{34}} - D_{\Gamma_{12}}^* \Gamma_{23}^* D_{\Gamma_{24}} D_{\Gamma_{34}}. \]

The Kraus generators are
\[ A_1 = \begin{bmatrix} L_{11} & \Gamma_{12} L_{22} \\ Z L_{33} & W L_{44} \end{bmatrix}, \quad A_2 = \begin{bmatrix} 0 \\ (D_{\Gamma_{12}} \Gamma_{23} - \Gamma_{12}^* \Gamma_{13} D_{\Gamma_{23}}) L_{33} \\ D_{\Gamma_{12}} L_{22} \end{bmatrix}, \]
\[ A_3 = \begin{bmatrix} 0 & 0 \\ D_{\Gamma_{13}} D_{\Gamma_{23}} L_{33} & Y L_{44} \end{bmatrix}, \quad A_4 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}. \]

The advantage is that, once the parameters of \( S_{\Phi} \) associated by Theorem 1 are known, the Cholesky factorization can be computed by (2.6). Indeed, the algorithms in the appendix for calculating the \( \Gamma_{kj} \), systematically compute a Cholesky factorization. Also, the orthogonality properties of the Cholesky factorization might be useful in some situations. These constructions make sense in infinite dimensions, except that further qualifications are needed for the trace-preserving property to be meaningful.

5. Appendix

In this appendix, a sketch of the proof of Theorem 1 is first given. This proof does not immediately yield a constructive procedure for finding the \( \Gamma_{kj} \). For that purpose, we next discuss briefly the notion of displacement structure (which works for a family of matrices with operator entries). A key feature of a displacement structure is that all possible Schur complements of such a family of matrices inherit a related displacement structure (this is what enables the determination of Cholesky factorizations of each member of the family). This is stated in Algorithm 8. We next show how any positive matrix can be imbedded into a family of matrices with displacement structure. Typically, a family with displacement structure admits more than one such representation. We choose one such representation - the specific choice for \( F(-t) \) enables the association of a lattice structure to the corresponding version of Algorithm 8. Now, if \( \mathcal{H} \) is of finite dimension, this specific choice of displacement structure made for positive matrices, results in a significant simplification of Algorithm 8. This is stated in Algorithm 9. In particular, a series of explicitly determined finite-dimensional contractions, \( \gamma_k(t) \), is produced by the algorithm. In terms of these, \( \gamma_k(t) \), there is a simple and explicit formula for the parameters, \( \Gamma_{kj} \). Thus, the determination of the parameters, \( \Gamma_{kj} \), is fully constructive when \( \mathcal{H} \) is finite dimensional (much of the procedure survives even when \( \mathcal{H} \) is infinite dimensional).

5.1. Parametrization of positive matrices. We now sketch a proof of Theorem 1. Since the diagonal entries of \( S \) intervene in the parametrization only through the \( L_{kk} \) (\( S_{kk} = L_{kk} \gamma_k \gamma_{kk} \)), we assume, without loss of generality, that \( S_{kk} = I_{\mathcal{H}} \) for all \( k = 1, \ldots, d \). By
a result of Kolmogorov (Theorem 1.3.1 in [4]), there exist a Hilbert space $\mathcal{K}$ containing $\mathcal{H}$ and isometries $V_k \in \mathcal{L}(\mathcal{H}, \mathcal{K}), k = 1, \ldots, d$, such that

(i) The set $\{V_k \mathcal{H} | k = 1, \ldots, d\}$ is total in $\mathcal{K};$

(ii) $S_{k,j} = V_k^* V_j, \quad k, j = 1, \ldots, d.$

Since $V_1$ is an isometry, we can identify $\mathcal{H}$ with the range of $V_1$ and assume $V_1 = P^K_{\mathcal{H}}$, where $P^K_{\mathcal{H}}$ denotes the orthogonal projection of $\mathcal{K}$ onto $\mathcal{H}$. Since $V_2$ is an isometry, there is a Hilbert space $\mathcal{D}_2$ and an operator $D_2 \in \mathcal{L}(\mathcal{D}_2, \mathcal{K})$ such that

$$W_1 = \begin{bmatrix} V_2 & D_2 \end{bmatrix} : \mathcal{H} \oplus \mathcal{D}_2 \to \mathcal{K}$$

is a unitary operator and $V_2 = W_1/\mathcal{H}$. Set $\mathcal{K}_1 = \mathcal{K}, \mathcal{K}_2 = \mathcal{H} \oplus \mathcal{D}_2$. By induction we obtain a family of unitary operators $W_1 \in \mathcal{L}(\mathcal{K}_2, \mathcal{K}_1), \ldots, W_{d-1} \in \mathcal{L}(\mathcal{K}_d, \mathcal{K}_{d-1})$ such that

$$V_k = W_1 \ldots W_{k-1}/\mathcal{H}, \quad k = 2, \ldots, d.$$

In particular,

$$S_{k,j} = P^K_{\mathcal{H}} W_k \ldots W_{j-1}/\mathcal{H}, \quad k < j. \tag{5.1}$$

Now, we notice that by a suitable identification of spaces,

$$W_1 = \begin{bmatrix} \Gamma_{12} & a & b \\
D_{12} & A_{11} & A_{12} \\
0 & A_{21} & A_{22} \end{bmatrix}.$$ 

Multiplying this operator on the left by the unitary operator $R(\Gamma_{12}) \oplus I$, we obtain a unitary operator with matrix representation

$$\begin{bmatrix} I & X & Y \\
0 & A'_{11} & A'_{12} \\
0 & A'_{21} & A'_{22} \end{bmatrix}.$$ 

It follows that necessarily, $X = 0$ and $Y = 0$. Iterating this construction and using (5.1) and (ii), we deduce (2.5).

5.2. Algorithms As discussed above, the notion of displacement structure is useful in producing an algorithmic procedure for finding the $\Gamma_{kj}$. The systematic study of the displacement structure was initiated in [10]. A main theme of the theory is the recursive factorization of matrices with implicit structure encoded by a so-called displacement equation of the form

$$R(t) - F(t)R(t - 1)F(t)^* = G(t)J(t)G(t)^*, \quad t \in \mathbb{Z}.$$ 

Given $R(t - 1)$, we need to know $\{F(t), G(t), J(t)\}$ in order to determine $R(t)$ using (5.2). We shall not seek to determine $R(t)$ by explicitly applying (5.2). Instead, we shall use the fact that $R(t)$ is a “low rank” modification of $R(t - 1)$ and exploit it to determine $R(t)$ more efficiently. This idea will operate as follows. Use as input data $\{F(t), G(t), J(t)\}$ and the Cholesky factor of $R(t - 1)$, say $\bar{L}(t - 1)$, and then compute the Cholesky factor of $R(t)$ without determining $R(t)$,

$$R(t) = \bar{L}(t)\bar{L}^*(t). \tag{5.3}$$
The following algorithm, see [6], tells us how to compute the columns of \( \bar{L}(t) \) from the columns of \( L(t-1) \) and knowledge of \{F(t), G(t), J(t)\}. Here we describe the algorithm for special types of \{F(t), G(t), J(t)\}, which subsume the case of positive-definite matrices \( R(t) \).

Let \( \bar{l}_k(t) \) denote the nonzero part of the \( k \)-th column of \( \bar{L}(t) \). Let also \( 1/\sqrt{d_k(t)} \) denote the top entry of \( \bar{l}_k(t) \) and define

\[
l_k(t) = \sqrt{d_k(t)} \bar{l}_k(t).
\]

That is, the top entry of \( l_k(t) \) is normalized to 1, and we also obtain the equivalent triangular factorization for \( R(t) \),

\[(5.4) \quad R(t) = L(t)D^{-1}(t)L^*(t),\]

where the diagonal entries of \( D(t) \) are the \{\( d_k(t) \)\} and the columns of \( L(t) \) are the \{\( l_k(t) \)\}. Here, \( L(t) \) is a unit diagonal lower triangular matrix. Let \( R_k(t) \) denote the Schur complement of \( R(t) \) with respect to its leading \( k \times k \) block. Suppose \( F(t) \) is lower triangular with diagonal entries \( f_k(t) \) and let \( F_k(t) \) denote the matrix obtained by deleting the first \( k \) rows and columns of \( F(t) \).

**Algorithm 8.** Assume we know

\[
\{L(t-1), D(t-1), G(t), F(t), J(t)\},
\]

and that \( R(t) \) satisfies the displacement equation \[(5.2).\] Then, for each \( k \), the Schur complements, \( R_k(t) \), of \( R(t) \) with respect to its leading \( k \times k \) block, satisfy similar displacement equations,

\[(5.5) \quad R_k(t) - F_k(t)R_k(t-1)F_k^*(t) = G_k(t)J(t)G_k^*(t),\]

where the \( G_k(t) \), and the triangular factorization \[(5.4) \] of \( R(t) \), can be obtained from the following recursive construction:

\[(5.6) \quad \begin{bmatrix} l_k(t) & 0 \\ G_{k+1}(t) \end{bmatrix} = \begin{bmatrix} F_k(t)l_k(t-1) & G_k(t) \\ F_k^*(t) & h_k^*(t)J_k(t) \end{bmatrix} \begin{bmatrix} f_k^*(t) & h_k^*(t)\Theta_k(t) \\ J(t)g^*_k(t) & p^*_k(t)\Theta_k(t) \end{bmatrix},\]

where \( g_k(t) \) is the top row of \( G_k(t) \), and \( h_k(t) \) and \( p_k(t) \) are chosen so as to satisfy the relation

\[
\begin{bmatrix} f_k(t) & g_k(t) \\ h_k(t) & p_k(t) \end{bmatrix} \begin{bmatrix} d_k(t-1) & 0 \\ 0 & J(t) \end{bmatrix} \begin{bmatrix} f_k(t) & g_k(t) \\ h_k(t) & p_k(t) \end{bmatrix}^* = \begin{bmatrix} d_k(t) & 0 \\ 0 & J(t) \end{bmatrix}.
\]

It is shown in [6] that it is always possible to find \( h_k(t) \) and \( p_k(t) \) as above. Choices that result in array (lattice) form descriptions are also possible and are described in detail in [6].
Displacement Structure for Positive Matrices

Let $S$ be positive. For $t = 0, \ldots, d - 1,$

$$R(-t) = \begin{bmatrix} I & S_{t+1,t+2} & S_{t+1,d} \\ S_{t+1,t+2}^* & I & S_{t+2,d} \\ \vdots & \vdots & \vdots \\ S_{t+1,d}^* & S_{t+2,d} & I \end{bmatrix} \oplus I \oplus \ldots \oplus I,$$

so that, $R(0) = S_\Phi$ and $R(-d + 1) = I \oplus \ldots \oplus I.$ Then, for $t = 0, \ldots, d - 1,$

$$F(-t) = F = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ I & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & I & \cdots & 0 \end{bmatrix}, \quad G(-t) = \begin{bmatrix} I & 0 \\ S_{t+1,t+2}^* & S_{t+1,t+2} \\ \vdots & \vdots \\ S_{t+1,d}^* & S_{t+1,d} \end{bmatrix},$$

and

$$J(-t) = J = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix}.$$

We easily check that

$$(5.7) \quad R(-t) - FR(-t - 1)F^* = G(-t)JG(-t)^*, \quad t = 1, \ldots, d - 2,$$

so that, $d - 2$ steps of Algorithm 8 will exploit the whole information encoded in $R(0) = S_\Phi.$

We notice that Algorithm 8 is greatly simplified with the special choice of $R(t), F(t), G(t),$ when $\mathcal{H}$ is of finite dimension. Thus, write $g_k(t) = [u_k(t) \ v_k(t)]$ with respect to the decomposition of $J$ and since $f_k(t) = 0,$ we deduce $d_k(t) = g_k(t)Jg_k(t)^* = u_k(t)u_k(t)^* - v_k(t)v_k(t)^*.$ The positivity of $S_\Phi$ is therefore tested by the condition $u_k(t)u_k(t)^* - v_k(t)v_k(t)^* \geq 0$ for all $t$ and all $k.$ If this holds for some $t$ and some $k,$ then there exist explicitly determined contractions, $\gamma_k(t),$ satisfying such that $v_k(t) = u_k(t)\gamma_k(t).$ In this situation we introduce

$$\Theta_k(t) = \begin{bmatrix} I & -\gamma_k(t) \\ -\gamma_k(t)^* & I \end{bmatrix} \begin{bmatrix} (I - \gamma_k(t)\gamma_k(t)^*)^{-1/2} & 0 \\ 0 & (I - \gamma_k(t)^*\gamma_k(t))^{-1/2} \end{bmatrix}$$

and then the generator recursion in Algorithm 8 reduces to a simpler form.

Algorithm 9. The generator recursion for the displacement equation (5.7) associated to a positive matrix $S$ has the form:

$$G_{k+1}(t) = FG_k(t - 1)\Theta_k(t - 1) \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix} + G_k(t)\Theta_k(t) \begin{bmatrix} 0 & 0 \\ 0 & I \end{bmatrix}.$$

Algorithm 9 produces an explicit connection between the parameters $\gamma_k(t)$ and the entries $S_{k,j}$ of $S.$ Namely, a direct calculation yields the following result.
Theorem 10. $\Gamma_{k,j} = \gamma_{j-k}(1-k)^*$, $1 \leq k < j \leq d$.

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