Interpolation for Completely Positive Maps: Numerical Solutions

by
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Abstract

We present a few techniques to find completely positive maps between full matrix algebras taking prescribed values on given data, based on semidefinite programming, convex minimization supported by a numerical example, as well as representations by linear functionals. The particular case of commutative data is also discussed.

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1 Introduction

The present paper refers to a certain interpolation problem for completely positive maps that take prescribed values on given matrices, closely related to problems recently considered by C.-K. Li and Y.-T. Poon in [27], Z. Huang, C.-K. Li, E. Poon, and N.-S. Sze in [19], T. Heinosaari, M.A. Jivulescu, D. Reeb, and M.M. Wolf in [17] as well as G.M. D'Ariano and P. Lo Presti [13], D.S. Gonçalves et al. [16].

Let M_n denote the C^*-algebra of all $n \times n$ complex matrices. In particular, positive elements (positive semidefinite matrices) in M_n are defined. Recall that a matrix $A \in M_n$ is *positive semidefinite* if all its principal determinants are nonnegative. Let $M_n^+ \subset M_n$ denote the convex cone of all such matrices. Set $M_n^h := \{A \in M_n : A^* = A\}$ where A^* denotes as usual the adjoint of A. A linear map $\varphi \colon M_n \to M_k$ is *positive* if $\varphi(M_n^+) \subset M_k^+$, namely it maps positive semidefinite matrices into positive semidefinite ones. Then $\varphi(A^*) = \varphi(A)^*$ for every $A \in M_n$. We call φ *completely positive* if $I_m \otimes \varphi \colon M_m \otimes M_n \to M_m \otimes M_k$ is positive for all $m \in \mathbb{N}$. An equivalent notion is that of *positive semidefinite* map, that is, for all $m \in \mathbb{N}$, all $h_1, \ldots, h_m \in \mathbb{C}^k$ and all $A_1, \ldots, A_m \in M_n$ we have $\sum_{i,j=1}^m \langle \varphi(A_j^* A_i) h_j, h_i \rangle \geq 0$. Let $\mathrm{CP}(M_n, M_k)$ denote the convex cone of all completely positive maps $\varphi \colon M_n \to M_k$. If $\varphi \colon M_n \to M_k$ is completely positive then, cf. K. Kraus [23] and M.D. Choi [12], there are $n \times k$ matrices $V_1, V_2, \ldots, V_m$ with $m \leq nk$ such that

$$\varphi(A) = V_1^* A V_1 + V_2^* A V_2 + \cdots + V_m^* A V_m \text{ for all } A \in M_n \tag{1.1}$$

(and, of course, any map of the form (1.1) is completely positive). The representation (1.1) is called the *Kraus representation* of φ and $V_1, \ldots, V_m$ are called the *operation elements*. The representation (1.1) of a given completely positive map φ is non-unique, however the minimal number of the operation elements in the Kraus form of such a map φ turns to be the rank of its Choi matrix Φ_φ, cf. [12]. The next problem was raised by C.-K. Li and Y.-T.

Poon in [27], where a solution was given in case of commutative families of matrices $(A_\nu)_\nu$, $(B_\nu)_\nu$.

Problem A. *Given matrices $A_\nu \in M_n$ and $B_\nu \in M_k$ for $\nu = 1, \ldots, N$, establish if there exist, and find $\varphi \in \mathrm{CP}(M_n, M_k)$ subject to the conditions*

$$\varphi(A_\nu) = B_\nu, \text{ for all } \nu = 1, \ldots, N. \tag{1.2}$$

Other linear affine restrictions on φ may be added as well, like trace preserving etc. We can assume all $A_\nu \in M_n^h$, $B_\nu \in M_k^h$ (write also $\varphi(A_\nu)^* = B_\nu^*$, replace A_ν by $A_\nu + A_\nu^*$ etc.).

In a first paper [5] we dealt with various necessary and/or sufficient conditions for the existence of solutions in terms of the *density matrix*, see our Theorems 2.4 and 2.5 in [5]. Most of results in this sense are related to Arveson's Hahn-Banach type theorem [2] and various techniques of operator spaces, some of which being simplified in the present particular context by R.R. Smith and J.D. Ward [30]. In this article, we focus on methods, based on the Choi matrix Φ_φ, that can be numerically implemented in an efficient way.

The first step in our approach is to firstly derive, in Subsection 2.1, an equivalent formulation in terms of existence of certain positive semidefinite matrices subject to linear affine restrictions, like the matrix $X \ (= \Phi_\varphi)$ in Problem B. If the trace preserving condition is added to Problem A, that is, if φ must be a *quantum channel*, this fits Problem B since the additional constrained is just another linear one. In Subsection 2.2 we remind a method to solve Problem B by known techniques of semidefinite programming. In Subsection 2.3 we present another technique for such problems, via results in [3] and based on convex minimization, namely (in case of Problem A with $A_\nu^* = A_\nu$ and $B_\nu^* = B_\nu$) of the function $\mathrm{tr}\left(e^{\sum_\nu A_\nu^\tau \otimes X_\nu}\right) - \mathrm{tr} \sum_\nu B_\nu X_\nu$ over all matrices $X_\nu \in M_k^h$ where τ denotes the transposition and "tr" stands for the trace, see Theorem 2.4, (a). A numerical example illustrating this technique is performed in Subsection 2.4. Finally, in Subsection 2.6 we show that, under the commutation assumptions, the semidefinite programming problem we obtain here turns into a linear programming one, hence explaining the results in [27] from our perspective.

Let us mention that the positive semidefinite approach to Problem A has been previously observed also in [13], [16] and [17], in different formulation. In particular, the feasibility of (1.2) in $\mathrm{CP}(M_n, M_k)$ was already known to be characterized [17] by the positivity of the functional $\sum_\nu A_\nu^\tau \otimes X_\nu \mapsto \mathrm{tr} \sum_\nu B_\nu X_\nu$ (statement recovered also by Theorem 2.4.(b)). With respect to the cited works, our main results by the convex minimization approach to Problem A in subsections 2.3 and 2.4, as well as other topics like propositions 2.7.(b) and 2.8, are new.

2   Main results

Consider then the interpolation problem (1.2) for the given matrices $A_\nu \in M_n$ and $B_\nu \in M_k$ where $\nu = 1, \ldots, N$. Firstly, we will translate it in terms of Choi matrices.

2.1   Equivalent setting of the problem

Let $\{e_i^{(n)}\}_{i=1}^n$ be the canonical basis of $\mathbb{C}^n$ ($n \in \mathbb{N}$). As usual, the linear space $M_{n,k}$ of all $n \times k$ matrices is identified with the vector space $\mathcal{B}(\mathbb{C}^k, \mathbb{C}^n)$ of all linear transformations $\mathbb{C}^k \to \mathbb{C}^n$ ($n, k \in \mathbb{N}$). Let $\{E_{i,m}^{(n,k)} \mid i = 1, \ldots, n, \ m = 1, \ldots, k\} \subset M_{n,k}$ be the matrix units

of size $n \times k$, namely $E_{i,m}^{(n,k)}$ is the $n \times k$ matrix with all entries 0 except for the (i,m)-th entry which is 1. If $n = k$, we note $E_{i,j}^{(n)} = E_{i,j}^{(n,n)}$.

Given any linear map $\varphi \colon M_n \to M_k$, define the $kn \times kn$ matrix Φ_φ, called the *Choi matrix*, see J. de Pillis [28], A. Jamiołkowski [20], R.D. Hill [18], and M.D. Choi [12], by

$$\Phi_\varphi = [\varphi(E_{i,j}^{(n)})]_{i,j=1}^n. \tag{2.1}$$

In what follows we use the description of the mapping $\varphi \mapsto \Phi_\varphi$ as in [14]: The formula

$$\varphi_{(i-1)k+m,(j-1)k+l} = \langle \varphi(E_{i,j}^{(n)})e_l^{(k)}, e_m^{(k)} \rangle, \quad i,j = 1,\ldots,k, \ l,m = 1,\ldots,n, \tag{2.2}$$

and its inverse $\varphi(C) = \sum_{r,s}^{nk} \varphi_{r,s} \mathcal{E}_r^* C \mathcal{E}_s$ for $C \in M_n$, establish a linear bijection

$$\mathcal{B}(M_n, M_k) \ni \varphi \mapsto \Phi_\varphi = [\varphi_{r,s}]_{r,s=1}^{nk} \in M_{nk} \tag{2.3}$$

that induces an affine, order preserving, continuous bijection between closed convex cones

$$\mathrm{CP}(M_n, M_k) \ni \varphi \mapsto \Phi_\varphi \in M_{nk}^+. \tag{2.4}$$

Consequently, the Choi matrix $\Phi = \Phi_\varphi$ of any solution $\varphi : M_n \to M_k$ to (1.2) is given by $\Phi = [\varphi_{r,s}]_{r,s}$ where the indices r, s are couples $r \equiv (i,m)$, $s \equiv (j,l)$ for $i,j = 1,\ldots,n$, $l,m = 1,\ldots,k$ and $\varphi_{r,s} = \langle \varphi(E_{i,j}^{(n)})e_l^{(k)}, e_m^{(k)} \rangle$. Since r, s run the cartesian product $\{1,\ldots,n\} \times \{1,\ldots,k\}$ consisting of nk elements, we can write $\Phi \in M_{nk}$ and $r,s = 1,\ldots,nk$. Set $A_\nu = [a_{\nu,i,j}]_{i,j=1}^n = \sum_{i,j=1}^n a_{\nu,i,j} E_{ij}^{(n)}$ and $B_\nu = [b_{\nu,m,l}]_{m,l=1}^k = \sum_{m,l=1}^k b_{\nu,m,l} E_{ml}^{(k)}$. Equate the (m,l) entries in the equality $\varphi(A_\nu) = B_\nu$ to get $\langle \varphi(A_\nu)e_l^{(k)}, e_m^{(k)} \rangle = b_{\nu,m,l}$, that is, $\langle \varphi(\sum_{i,j=1}^n a_{\nu,i,j} E_{ij}^{(n)})e_l^{(k)}, e_m^{(k)} \rangle = b_{\nu,m,l}$ and so

$$\sum_{i,j=1}^n a_{\nu,i,j} \varphi_{(i,m)(j,l)} = b_{\nu,m,l}. \tag{2.5}$$

Write the equality from above using Kronecker's symbol $\delta_{p,q}$ ($= 1$ if $p = q$ and 0 if $p \neq q$) as $\sum_{(j,l'),(i,m')} a_{\nu,i,j} \delta_{l',l} \delta_{m',m} \varphi_{(i,m')(j,l')} = b_{\nu,m,l}$ where (j,l') and (i,m') run $\{1,\ldots,n\} \times \{1,\ldots,k\}$, then set

$$c(\nu,m,l)_{(j,l')(i,m')} := a_{\nu,i,j} \delta_{l',l} \delta_{m',m} = (A_\nu^\tau)_{j,i}(E_{l,m}^{(k)})_{l',m'} = (A_\nu^\tau \otimes E_{l,m}^{(k)})_{(j,l'),(i,m')} \tag{2.6}$$

and define

$$C(\nu,m,l) = \left[c(\nu,m,l)_{(j,l')(i,m')}\right]_{(j,l')(i,m')} = A_\nu^\tau \otimes E_{lm}^{(k)} \tag{2.7}$$

that can be represented as an $nk \times nk$ matrix $C(\nu,m,l) \in M_{nk}$

$$C(\nu,m,l) \equiv A_\nu^\tau \otimes E_{l,m}^{(k)} \equiv \left[a_{\nu,j,i} E_{l,m}^{(k)}\right]_{i,j=1}^n \tag{2.8}$$

via the linear, isometric, order-preserving isomorphisms of C^*-algebras $M_{nk} \equiv M_n \otimes M_k \equiv M_n(M_k)$. We obtain, using (2.5) – (2.7), $\sum_{(j,l'),(i,m')} c(\nu,m,l)_{(j,l')(i,m')} \varphi_{(i,m')(j,l')} = b_{\nu,m,l}$, namley $\mathrm{tr}\,(C(\nu,m,l)\Phi) = b_{\nu,m,l}$, that by (2.8) we can write as well

$$\mathrm{tr}\left[(A_\nu^\tau \otimes E_{l,m}^{(k)})\Phi\right] \ \left(= \mathrm{tr}\left[(A_\nu \otimes E_{m,l}^{(k)})\Phi^\tau\right]\right) = b_{\nu,m,l}. \tag{2.9}$$

This actually is a particular application of the next formula, easily checked following the lines from above, letting $A = [a_{i,j}]_{i,j=1}^n = \sum_{i,j=1}^n a_{i,j} E_{i,j}^{(n)}$ etc.:

$$\varphi(A) = \left[\operatorname{tr}\left[(A^\tau \otimes E_{l,m}^{(k)})\Phi\right]\right]_{m,l=1}^k = \left[\operatorname{tr}\left[(A \otimes E_{m,l}^{(k)})\Phi^\tau\right]\right]_{m,l=1}^k \quad (A \in M_n). \tag{2.10}$$

Note that we have as well the formula $\varphi(A) = [\operatorname{tr}\left[(E_{l,m}^{(k)} \otimes A)D_\varphi^*\right]_{m,l=1}^k$ where D_φ denotes the density matrix [5], for which we also omit the details. Conditions (2.2) on φ are thus equivalent to the equations (2.9) from above concerning Φ, via the formulas (2.6), (2.7) and (2.2), (2.3). Denote by $\iota = (\nu, m, l)$ the generic triple consisting of arbitrary $\nu = 1, \ldots, N$ and $m, l = 1, \ldots, k$. Thus ι runs a set of $q := Nk^2$ elements. We may write $\iota = 1, \ldots, q$. Set also $p = nk$. Write $C(\iota) = C(\nu, m, l)$ $(\in M_p)$ and $b_\iota = b_{\nu,m,l}$; denote Φ by X, below.

With these notations, via (2.4) Problem A takes then the equivalent form from below.

Problem B *Given $C(\iota) \in M_p$ and numbers b_ι $(1 \leq \iota \leq q)$, find $X \in M_p$, $X \geq 0$, such that*

$$tr\,(C(\iota)X) = b_\iota \quad for \; all \; \iota = 1, \ldots, q. \tag{2.11}$$

Thus, the solvability of Problem A leads to the rather known topic of finding positive semidefinite matrices subject to linear affine conditions and, in particular, establishes whether such matrices do exist. These questions often occur and are dealt with by reliable numerical methods in the semidefinite programming, a few elements of which we sketch in what follows.

2.2 Solutions by means of semidefinite programming

Firstly, using $\operatorname{tr}(c^*) = \overline{\operatorname{tr}(c)}$, $\operatorname{tr}(cd) = \operatorname{tr}(dc)$ and writing equation (2.11) in terms of $C(\iota) + C(\iota)^*$ and $i(C(\iota) - C(\iota)^*)$ we can asume all matrices $C(\iota)$ to be selfadjoint. We can suppose, without loss of generality, that they are linearly independent over $\mathbb{R}$. *Semidefinite programming* is concerned with minimization of linear functionals subject to the constraint that an affine combination of selfadjoint matrices is positive semidefinite: see in this sense [7], [9], [24], [26], [31], also [10], [15]. Roughly speaking, one sets $a(x) = \sum_\iota x_\iota C(\iota) + a_0$ for the given $C(\iota)$ and a selfadjoint matrix a_0 that can be suitably chosen, here. Define then $p^* = \inf_x\{\sum_\iota b_\iota x_\iota : a(x) \geq 0\}$ and $q^* = \inf_X\{-\operatorname{tr}(a_0X) : X \geq 0, \operatorname{tr}(C(\iota)X) = b_\iota \,\forall\iota\}$. A problem dual to (2.11) occurs now with respect to p^*, namely to establish if there exist positive definite matrices of the form $a(x)$. Standard algorithms exist to this aim, based on maximizing the minimal eigenvalue of $a(x)$ in the variables $x = (x_\iota)_\iota$, or on interior point methods using barrier functions [26]. In the case when either (2.11) has solutions $X > 0$, or the dual problem has solutions x with $a(x) > 0$, we have $p^* = q^*$, see for instance [26], [31]. If both conditions hold, the optimal sets for p^* and q^* are nonempty. In this case for every $\lambda \in (p^*, \bar{p})$ where $\bar{p} = \sup_x\{\sum_\iota b_\iota x_\iota : a(x) > 0\}$ there is a unique vector $x^* = (x_\iota^*)_\iota$, the *analytic center* of this linear matrix inequality, such that $a(x^*) > 0$, $\sum_\iota b_\iota x_\iota^* = \lambda$ and x^* minimizes the *logarithmic barrier function* $\ln \det a(x)^{-1}$ over all x with $\sum_\iota b_\iota x_\iota$ and $a(x) > 0$. It follows by the Lagrange multipliers method that $\operatorname{tr}(C(\iota)a(x^*)^{-1}) = \lambda b_\iota \,\forall\iota$, which gives a solution $X = X_*$ of (2.11), namely $X_* = \lambda^{-1}a(x^*)^{-1}$.

2.3 Solutions via a convex minimization technique

We show how to obtain solutions to Problems A, B by minimizing a certain convex function. Let $C(\iota) \in M_p$ denote now arbitrary selfadjoint and linearly independent matrices and b_ι

some real numbers for $\iota = 1, \ldots, q$. Define the function V of q real variables $x = (x_\iota)_\iota$ by

$$V(x) = \operatorname{tr}\left(e^{\sum_{\iota=1}^{q} x_\iota C(\iota)}\right) - \sum_\iota x_\iota b_\iota. \tag{2.12}$$

Then V is smooth, strictly convex, with strictly positive definite Hessian. Hence if it has a critical point this is unique, and necessarily a minimum. Generally we may have also an unattained infimum $\inf V > -\infty$, or $\inf V = -\infty$. For details see [3] (where V occurs by maximizing $-\operatorname{tr}(X \ln X)$ subject to equations of the form (2.11), which holds for an X given by (2.13)). In the next result we characterize the existence of solutions $X > 0$ to Problem B.

Theorem 2.1. [3]. *The system of equations* $\operatorname{tr}(C(\iota)X) = b_\iota$ $(\iota = 1, \ldots, q)$ *admits solutions* $X > 0$ *if and only if the function* V *defined by (2.12) has a critical point (of minimum), that is, if and only if* $\lim_{x \to \infty} V(x) = +\infty$. *In this case, if* $x^0 = (x_\iota^0)_\iota$ *denotes the critical point of* V, *we have also the (positive) particular solution*

$$X_0 = e^{\sum_\iota x_\iota^0 C(\iota)}. \tag{2.13}$$

Remark 2.2. (a) The function V given by (2.12) fulfills the conditions of application of the *method of the conjugate gradients* [11]. This yields, if problem (2.11) has solutions $X > 0$, a minimizing sequence of vectors $x = (x_\iota)_\iota$ that is convergent to the critical point x^0 and so provides approximations $\widetilde{X}_0 = e^{\sum_\iota x_\iota C(\iota)} \approx X_0$ of the solution (2.13), see Example 12 and Remark 11 in [3]. The gradient $\nabla V = (\partial V / \partial x_\iota)_{\iota=1}^q$ of V is easily computed to this aim by $\frac{\partial V}{\partial x_\kappa}(x) = \operatorname{tr}(C(\kappa) e^{\sum_\iota x_\iota C(\iota)}) - b_\kappa$, see [3]. Various versions of Newton's method that can be used as well to approximate x^0.

(b) In the particular case of our Problem A and for selfadjoint data, after replacing the matrices $C = C(\nu, m, l) = A_\nu^\tau \otimes E_{l,m}$ by the symmetrized ones $C + C^*$ etc. as described at the beginning of Subsection 2.3, setting $X_\nu = [x_{\nu,m,l} + \overline{x}_{\nu,l,m}]_{l,m=1}^k \in M_k$ the function V becomes

$$V((x_\nu)_\nu) = \operatorname{tr}\left(e^{\sum_{\nu=1}^{N} A_\nu^\tau \otimes X_\nu}\right) - \operatorname{tr} \sum_\nu B_\nu X_\nu \tag{2.14}$$

since in this case $\sum_\iota x_\iota C(\iota) = \sum_\nu A_\nu^\tau \otimes X_\nu$ and $\sum_\iota b_\iota x_\iota = \operatorname{tr} \sum_\nu B_\nu X_\nu$. Differentiating the right hand side of (2.14) obviously shows now that a critical point $(X_\nu)_\nu$ provides a solution φ of (1.2) via formula (2.10) in which $\Phi = \Phi_\varphi = e^{\sum_\nu A_\nu \otimes X_\nu^\tau}$.

(c) A test [3] exists to check if the system $\operatorname{tr}(C(\iota)X) = b_\iota$ has no solutions $X \geq 0$ at all, too, namely $\inf V = -\infty$ in which case the minimization provides, after some iterations, vectors $x = (x_\iota)_\iota$ such that $\sum_\iota x_\iota C(\iota) \geq 0$ but $\sum_\iota b_\iota x_\iota < 0$ (see also Proposition 2.7.(a)). This also has a corresponding consequence for Problem A.

Remark 2.3. All approximations from a small neighborhood of the critical point of V can provide exact solutions X to Problem B as follows: fix a linear affine projection π onto the linear submanifold of M_p^h defined by the equations (2.11) and $X^* = X$, then for an approximation $\widetilde{X}_0$ of X_0 use $X := \pi \widetilde{X}_0$ instead of $\widetilde{X}_0$: since $\widetilde{X}_0 \approx X_0$, $X = \pi \widetilde{X}_0 \approx \pi X_0 = X_0$ and so $X \approx X_0 (> 0)$ which implies $X > 0$ if the approximation $\widetilde{X}_0 \approx X_0$ was good enough.

We summarize below the main topics stated in this Subsection.

Theorem 2.4. *Let $A_\nu \in M_n$ and $B_\nu \in M_k$ for $\nu = 1, \ldots, N$ be selfadjoint matrices. Let $\mathbb{V}$ be the (strictly convex, smooth, real) function defined by*

$$\mathbb{V}((X_\nu)_\nu) = tr\left(e^{\sum_{\nu=1}^{N} A_\nu^\tau \otimes X_\nu}\right) - tr \sum_\nu B_\nu X_\nu$$

on the real linear space of all sets $(X_\nu)_{\nu=1}^N$ consisting of selfadjoint matrices $X_\nu \in M_k$.

(a) *The following two statements are equivalent:*

(i) *Problem A has at least one solution φ from the (dense) interior of $\mathrm{CP}(M_n, M_k)$;*

(ii) *Function $\mathbb{V}$ has a (unique) critical point, namely its infimum $\inf \mathbb{V}$ is finite and attained. In this case the critical point $(X_\nu^0)_\nu$ provides, by formula (2.10), a particular solution φ_0 of (1.2) whose Choi matrix $\Phi = \Phi_{\varphi_0}$ is given by $\Phi = e^{\sum_\nu A_\nu \otimes (X_\nu^0)^\tau}$ (> 0). Moreover, all close enough sets $(X_\nu)_\nu \approx (X_\nu^0)_\nu$ provide solutions φ with $\Phi_\varphi = \pi(e^{\sum_\nu A_\nu \otimes (X_\nu)^\tau})$ as in Remark 2.3.*

(b) *The lack of any solution $\varphi \in \mathrm{CP}(M_n, M_k)$ of (1.2) is characterized by the condition $\inf \mathbb{V} = -\infty$, that is equivalent also to the existence of sets $(X_\nu)_\nu$ (some of which being always obtained when minimizing $\mathbb{V}$) such that $\sum_\nu A_\nu^\tau \otimes X_\nu \geq 0$ and $tr \sum_\nu B_\nu X_\nu < 0$.*

For (a), use Theorem 2.1 together with Remark 2.2.(b). Note to this aim that the mapping (2.4) is one-one between the interiors of the closed convex cones $\mathrm{CP}(M_n, M_k)$ and M_{nk}^+. For (b), use the results in [3] mentioned in Remark 2.2.(c).

2.4   A Numerical Example

We show how Theorem 2.4 applies to Problem A. Suppose one wishes to find $\varphi : M_2 \to M_2$ completely positive such that $\varphi(A_\nu) = B_\nu$ ($\nu = 1, 2$) for $A_1 = \begin{bmatrix} 2 & 1 \\ 1 & 0 \end{bmatrix}, A_2 = \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}$ and $B_1 = \begin{bmatrix} 4 & 0 \\ 0 & 0 \end{bmatrix}, B_2 = \begin{bmatrix} 3.5 & 1.5 \\ 1.5 & 2.5 \end{bmatrix}$. Use to this aim the minimization method indicated by Remark 2.2. Formulas (2.6), (2.7) and (2.8) provide the matrices $C(\iota)$ for $\iota = (\nu, m, l)$ where $\nu, m, l = 1, 2$. Due to the symmetry equation (2.5) (or, equivalently, (2.11)) is equivalent to $\sum_{j,i=1}^n \bar{a}_{\nu,ji} \bar{\varphi}_{(j,l)(i,m)} = \bar{b}_{\nu lm}$ (or $\mathrm{tr}\,(C(\iota)^* \Phi) = \bar{b}_\iota$), and so it is enough to consider (2.5) for those couples (m, l) with $m \leq l$. That is, for each $\nu = 1, 2$ we have 3 equations corresponding to $(m, l) = (1, 1), (1, 2), (2, 2)$. The set $\{1, 2\} \times \{1, 2\}$ of indices r, s like $(j, l), (j, l'), (i, m), (i, m')$ with $1 \leq i, j \leq n\,(= 2)$ and $1 \leq m, m', l, l' \leq k\,(= 2)$ from below is ordered lexicographically as $\{(1, 1), (1, 2), (2, 1), (2, 2)\} \equiv \{\mathbf{1, 2, 3, 4}\}$. We represent the positive matrix $X = [y_{\alpha,\beta}]_{\alpha,\beta \in \{\mathbf{1,2,3,4}\}} \equiv \Phi = [\varphi_{r,s}]_{r,s}$ that we seek for and the given matrices $C(\nu, m, l)$ as follows: $C(1, 1, 1) = A_1^\tau \otimes E_{111}$, $C(1, 1, 2) = A_1^\tau \otimes E_{2,1}$, etc. Numerically minimizing V gave us the matrix $\widetilde{X}_0 \approx X_0$,

$$\widetilde{X}_0 = \begin{bmatrix} 1.549937761 & -0.1694804138 & 0.4499571618 & 0.4047411695 \\ -0.1694804138 & 0.1534277390 & -0.06572393508 & -0.1533566973 \\ 0.4499571618 & -0.06572393508 & 0.5249880063 & 0.6652436210 \\ 0.4047411695 & -0.1533566973 & 0.6652436210 & 1.326699194 \end{bmatrix}$$

which is positive and approximately satisfies (2.11). Let φ be the map whose Choi matrix $\Phi = \Phi_\varphi = [\varphi_{r,s}]_{r,s}$ is $\widetilde{X}_0 \equiv \Phi$. We got then an approximate solution to our present particular case of problem (1.2), namely $\varphi(A) = \left[\sum_{i,j=1}^2 \Phi_{(i,m)(j,l)} a_{i,j}\right]_{m,l=1}^2 = \left[\mathrm{tr}[(A^\tau \otimes E_{lm}^{(2)})\widetilde{X}_0]\right]_{m,l=1}^2$

for every $A = [a_{i,j}]_{i,j=1}^2 \in M_2$, see formula (2.10) (or (2.9)). For instance, we have $\varphi(A_1)_{1,1} = \text{tr}\,(C(1,1,1)\widetilde{X}_0) = 2(\widetilde{X}_0)_{1,1} + (\widetilde{X}_0)_{1,3} + (\widetilde{X}_0)_{3,1} = 3.99978984 \approx 4 = (B_1)_{1,1}$, and $\varphi(A_1)_{1,2} = \text{tr}\left[(A_1^\tau \otimes E_{2,1}^{(2)})\widetilde{X}_0\right] = \text{tr}(C(1,1,2)\widetilde{X}_0) = 0.0000564069 \approx 0 = (B_1)_{1,2}$, etc.

Remark 2.5. Semidefinite programming methods [26], [31] (or related, as in Subsection 2.4) can solve problems of type B for more sizeable dimensions p $(= nk)$ and q $(= Nk^2)$, and so allow to consider Problem A as well for somewhat larger integers n, k, N. The difficulty is to compute the (trace of the) exponential for the matrix $\sum_\iota x_\iota C(\iota) \in M_p$ (or its determinant, in the semidefinite programming approach) required for V and ∇V. Common techniques to this aim like eigenvalue decomposition require a time of order p^3. We need just linear functionals of this exponential, for which stochastic methods exist requiring a time $\sim p^2$, but they are better only for very large p and provide rougher approximations [25]. See also [8], [22] for quantitative and software topics on the practicability range of the present methods.

Remark 2.6. Another question is to reduce the number of operation elements in the representation (1.1) of the solution φ of (1.2), whenever possible — that is, to minimize the rank of X in (2.11). The case of one term for instance corresponds to solutions $X \geq 0$ of rank one, namely to the existence of vectors $v \in \mathbb{C}^{nk}$ such that $\langle C(\iota)v, v \rangle = b_\iota$ for all ι. A first easy step to rank reduction is to find the joint support P of the symmetrizations $C = C(\iota) + C(\iota)^*$ etc. of the $C(\iota)$'s and consider solutions X such that $X = PXP$. Indeed, set $K = \{h \in \mathbb{C}^{nk} : Ch = 0 \forall C\}$. Let P be the orthogonal projection onto $K^\perp$. Then $C = CP$ and so $C = C^* = PC = PCP$, whence $\text{tr}\,(CX) = \text{tr}\,(PCPX) = \text{tr}\,(CPXP)$. Generally the question is difficult, for some possibilities of reducing the rank of X see for instance Section II.13 in [7], or [6], [29].

2.5 Characterization in terms of linear functionals

By Theorem 2.5 from [5] or [30]), the solvability of (2.11) is described in terms of the map $\sum_\iota x_\iota C(\iota) \mapsto b_\iota x_\iota$. We recall this result in the form from below, completed with a version (b) concerning the existence of strictly positive solutions; for the sake of completeness we sketch also the proof.

Proposition 2.7. *Suppose that $C(\iota) \in M_p$ $(\iota = 1, \ldots, q)$ are selfadjoint, linearly independent and their linear span contains strictly positive matrices. Then:*

(a) There exist solutions $X \geq 0$ of the system of equations (2.11) if and only if $\sum_\iota b_\iota x_\iota \geq 0$ for all $(x_\iota)_\iota$ such that $\sum_\iota x_\iota C(\iota) \geq 0$, namely, $\inf_{x\,:\,\sum_\iota x_\iota C(\iota) \geq 0} \sum_\iota b_\iota x_\iota \geq 0$.

(b) There exist solutions $X > 0$ of the system of equations (2.11) if and only if $\sum_\iota b_\iota x_\iota > 0$ for all $(x_\iota)_\iota \neq 0$ such that $\sum_\iota x_\iota C(\iota) \geq 0$, namely, $\inf_{x\,:\,\sum_\iota x_\iota C(\iota) \geq 0, \|x\|=1} \sum_\iota b_\iota x_\iota > 0$.

Proof. (a) Assume that $\inf_{x\,:\,\sum_\iota x_\iota C(\iota) \geq 0} \sum_\iota b_\iota x_\iota \geq 0$. The intersection of the closed convex cone of all positive semidefinite $p \times p$ matrices and the linear span S of the $C(\iota)$'s contains a point that is interior to the cone, namely a positive matrix. The linear functional $l :$ $\sum_\iota x_\iota C(\iota) \mapsto \sum_\iota b_\iota x_\iota$ is well defined, and ≥ 0 on this intersection. By Mazur's theorem, see for instance [1], [21], it has a linear extension L to the space M_p^s of all selfadjoint matrices in M_p, such that $LY \geq 0$ for all $Y \geq 0$ in M_p^s. Now L has the form $LY = \text{tr}\,(XY)$ for some $X \in M_p^s$. Letting $Y = \langle \cdot, h \rangle h$ for an arbitrary vector $h \in \mathbb{C}^p$ gives $\langle Xh, h \rangle \geq 0$.

Hence $X \geq 0$. Since $L|_S = l$, for every ι we have $C(\iota) \in S$ and $\mathrm{tr}\,(C(\iota)X) = LC(\iota) = lC(\iota) = b_\iota$. Conversely, suppose that there exists an $X \geq 0$ such that $\mathrm{tr}\,(C(\iota)X) = b_\iota$ for all ι. Then for every $(x_\iota)_\iota$ such that $\sum_\iota x_\iota C(\iota) \geq 0$, we have $\sum_\iota b_\iota x_\iota = \sum_\iota \mathrm{tr}\,(C(\iota)X)x_\iota = \mathrm{tr}\,(X \sum_\iota x_\iota C(\iota)) = \mathrm{tr}\,(X^{1/2} \sum_\iota x_\iota C(\iota)X^{1/2}) \geq 0$.

(b) Assume that $\inf_{x\,:\,\sum_\iota x_\iota C(\iota) \geq 0,\, \|x\|=1} \sum_\iota b_\iota x_\iota > 0$ ($\|\ \|$ is any norm). Proceed as above, except we need the following fact: given a finite dimensional real space M, a linear subspace S and a closed convex cone $C \subset M$ such that $C \cap (-C) = \{0\}$, any linear functional l on S such that $ls > 0$ for all $s \neq 0$ from $S \cap C$ has a linear extension L to M such that $Lm > 0$ for all $m \neq 0$ from C. This is rather a known consequence of the Hahn-Banach, Mazur - type theorems, see for instance [4]. The necessity follows as in the case (a). $\qquad\square$

2.6 The case of commutative data

In this case Problem A was shown by Theorem 2.1 in [27] to be equivalent to solving a system of nonhomogeneous linear equations in nonnegative variables. This result can be explained from the present perspective, too. Firstly, by the commutativity assumption we can suppose without loss of generality that all A_ν, B_ν are diagonal. For any matrix $u = [u_{ij}]_{i,j}$, set $\tilde{u} = [u_{ij}\delta_{i,j}]_{i,j}$. Then by Proposition 2.8, in the equations (2.9) we can replace any positive semidefinite Φ ($= C_\varphi$ for a solution φ of (1.2)) by the (positive semidefinite) diagonal matrix $\tilde{\Phi}$ ($= C_\psi$ for another solution ψ). This leads indeed to the problem of finding nk nonnegative numbers, namely the diagonal entries of $\tilde{\Phi}$, satisfying the system of Nk equations: $\mathrm{tr}\,[(A_\nu \otimes E_{l,l}^{(k)})\tilde{\Phi}] = B_{\nu,l,l}$ for $1 \leq \nu \leq N$ and $1 \leq l \leq k$.

Proposition 2.8. *If A_ν, B_ν are diagonal, $X \in M_{nk}$ and $tr\,[(A_\nu \otimes E_{m,l}^{(k)})X] = B_{\nu,l,m}$, then we have also the equality $tr\,[(A_\nu \otimes E_{m,l}^{(k)})\tilde{X}] = B_{\nu,l,m}$ (both terms of which are null if $m \neq l$).*

Proof. Represent $X \in M_{nk} \equiv M_n \otimes M_k$ as $X = \sum_\mu Y_\mu \otimes Z_\mu$ with $Y_\mu \in M_n$ and $Z_\mu \in M_k$. Using the easily checked formula $\widetilde{u \otimes v} = \tilde{u} \otimes \tilde{v}$, we obtain $\tilde{X} = \sum_\mu \tilde{Y}_\mu \otimes \tilde{Z}_\mu$. Hence, the equality in the conclusion holds for $l \neq m$ by inserting $\tilde{X}$ in the left hand side, then using the formula $\mathrm{tr}(u \otimes v) = \mathrm{tr}(u)\,\mathrm{tr}(v)$ and the equalities $\mathrm{tr}\,(E_{l,m}^{(k)}\tilde{Z}_\mu) = 0$, $B_{\nu,l,m} = 0$. To prove it also for $l = m$, use again $\mathrm{tr}(u \otimes v) = \mathrm{tr}\,u\,\mathrm{tr}\,v$ to write the desired conclusion in the form $\sum_\mu \mathrm{tr}\,(A_\nu \tilde{Y}_\mu)Z_{\mu,l,l} = B_{\nu,l,l}$. This is equivalent, by means of the equalities $\tilde{A}_\nu = A_\nu$ and the formula $\mathrm{tr}\,(\tilde{u}\tilde{v}) = \mathrm{tr}(\tilde{u}v)$, to $\mathrm{tr}\,[(A_\nu \otimes E_{ll}^{(k)}) \sum_\mu Y_\mu \otimes Z_\mu] = B_{\nu,l,l}$, that is the case $l = m$ of (2.9) and so holds true by hypotheses. $\qquad\square$

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