On the implementation of symmetric extensions

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Notation. — We work with finite Hilbert spaces. For a Hilbert space $\mathcal{H}$ of dimension d, $\mathsf{Lin}(\mathcal{H})$ is the set of linear operators on $\mathcal{H}$, while $\mathsf{Herm}(\mathcal{H}) = \{\sigma \in \mathsf{Lin}(\mathcal{H}) \text{ s.t. } \sigma = \sigma^*\}$ is the set of Hermitian operators, where σ^* denotes the adjoint of σ. Semidefinite positive operators are written $\mathsf{Herm}_+(\mathcal{H}) = \{\sigma \in \mathsf{Herm}(\mathcal{H}) \text{ s.t. } \forall|\varphi\rangle \in \mathcal{H}, \langle\varphi|\sigma|\varphi\rangle \geqslant 0\}$.

This last condition, $\forall|\varphi\rangle \in \mathcal{H}, \langle\varphi|\sigma|\varphi\rangle \geqslant 0$ is written more compactly $\sigma \succcurlyeq 0$.

By the existence of the finite computational basis, we can write indifferently $|\varphi\rangle \in \mathcal{H}$ or $\vec{\varphi} \in \mathbb{C}^d$; we also write $X \in \mathsf{Lin}(\mathcal{H})$ or $X \in \mathbb{C}^{d \times d}$.

1 Approximations of the separable cone

Let $\mathcal{H}_{\mathrm{A}} = \mathbb{C}^{d_{\mathrm{A}}}$ and $\mathcal{H}_{\mathrm{B}} = \mathbb{C}^{d_{\mathrm{B}}}$ two finite Hilbert spaces of dimension d_{A}, d_{B}.

Definition 1. *The* separable cone $\mathsf{Sep}(\mathcal{H}_A|\mathcal{H}_B)$ *contains the Hermitian operators* $\sigma \in \mathsf{Herm}(\mathcal{H}_A \otimes \mathcal{H}_B)$ *that possess a separable decomposition: there is a finite number of weights* $p_i \geqslant 0$*, states* $|\alpha_i\rangle \in \mathcal{H}_A$ *and* $|\beta_i\rangle \in \mathcal{H}_B$ *such that*

$$\sigma = \sum_i p_i |\alpha_i\rangle\langle\alpha_i| \otimes |\beta_i\rangle\langle\beta_i|. \tag{1}$$

Separable states, for example, are such that $\rho \in \mathsf{Sep}(\mathcal{H}_{\mathrm{A}}|\mathcal{H}_{\mathrm{B}})$ and $\mathrm{tr}[\rho] = 1$; however, our definition of $\mathsf{Sep}(\mathcal{H}_{\mathrm{A}}|\mathcal{H}_{\mathrm{B}})$ also include subnormalized states, or states with $\mathrm{tr}[\rho] > 1$.

An entanglement witness is an operator $W \in \mathsf{Herm}(\mathcal{H}_{\mathrm{A}} \otimes \mathcal{H}_{\mathrm{B}})$ such that $\mathrm{tr}[W\,\sigma] \geqslant 0$ for all $\sigma \in \mathsf{Sep}(\mathcal{H}_{\mathrm{A}}|\mathcal{H}_{\mathrm{B}})$. Thus, the cone of all such operators is the dual to $\mathsf{Sep}(\mathcal{H}_{\mathrm{A}}|\mathcal{H}_{\mathrm{B}})$.

However, deciding whether "$\rho \in \mathsf{Sep}(\mathcal{H}_{\mathrm{A}}|\mathcal{H}_{\mathrm{B}})$" is hard [?]. Instead, we consider an outer approximation $\tilde{\mathsf{S}} \supseteq \mathsf{Sep}(\mathcal{H}_{\mathrm{A}}|\mathcal{H}_{\mathrm{B}})$ containing all ρ possessing a k-symmetric extension τ, where k is the number of copies of the $\mathcal{H}_{\mathrm{B}}$ considered (precise definition below).

Optionally, we can require τ to have positive partial transpose (PPT), where the transpose is taken over a number c of copies of the B subsystem (a precise definition will follow). Several PPT constraints can be present at the same time, each corresponding to a number $1 \leqslant c_i \leqslant k$.

The approximation $\tilde{\mathsf{S}}$ is fully specified by the number k of copies of $\mathcal{H}_{\mathrm{B}}$ and the set $C = \{c_i\}$ defining the PPT constraints.

Definitions in the litterature. — The original paper by Doherty et al. [?] uses either $C = \emptyset$ or the full set of PPT constraints $C = \{1, \ldots, k\}$. Subsequent works by Navascués et al. [?, ?], however, use either $C = \emptyset$ or $C = \{\mathrm{ceil}(k/2)\}$ where $\mathrm{ceil}(x)$ is the smallest integer $\geqslant x$. **VERIFY** This incomplete PPT constraint is motivated by the definition of *inner* approximations of $\mathsf{Sep}(\mathcal{H}_{\mathrm{A}}|\mathcal{H}_{\mathrm{B}})$, which we do not study in the present note.

The toolbox QETLAB [?] uses this last convention, with either $C = \emptyset$ or $C = \{\mathrm{ceil}(k/2)\}$. **VERIFY**

We now precise the required notions.

1.1 Mathematical definitions

Definition 2. (Doherty [?]) *The operator* $\sigma \in \mathsf{Herm}(\mathcal{H}_A \otimes \mathcal{H}_B)$ *has a k-symmetric extension if there exists a semidefinite positive operator* $\tau \in \mathsf{Herm}_+(\mathcal{H}_A \otimes \mathcal{H}_{B_1} \otimes \ldots \otimes \mathcal{H}_{B_k})$ *such that:*

- *when restricted to* $\mathcal{H}_A \otimes \mathcal{H}_{B_1}$ *by the partial trace,* τ *reproduces* σ*:*

$$\mathrm{tr}_{B_2 \ldots B_k}[\tau] = \sigma, \tag{2}$$

  and the partial trace is defined by

$$\mathrm{tr}_{B_2 \ldots B_k}[\tau] = \sum_{j_2 \ldots j_k} [\mathbb{1}_A \otimes \mathbb{1}_{B_1} \otimes \langle j_2 \ldots j_k|]\, \tau\, [\mathbb{1}_A \otimes \mathbb{1}_{B_1} \otimes |j_2 \ldots j_k\rangle], \tag{3}$$

- *symmetry, first variant:* τ *is symmetric under all permutations of* $\mathcal{H}_{B_1} \otimes \ldots \otimes \mathcal{H}_{B_k}$*,*

- *symmetry, second variant: the support and range of* τ *is entirely contained in* $\mathcal{H}_A$ *and the symmetric subspace of* $\mathcal{H}_{B_1} \otimes \ldots \otimes \mathcal{H}_{B_k}$*.*

Let us clarify the notions used in this definition. The first variant uses the following.

Definition 3. *Let* $\pi \in \mathcal{S}_k$ *be an element of the symmetric group of degree k. Alternatively, let* $\{\pi_1, \ldots, \pi_k\}$ *be a set such that the integers* $1 \ldots. k$ *appear exactly once.*

The permutation operator P_π *associated to* π *is given by:*

$$P_\pi = \sum_{i j_1 \ldots j_k} |i j_{\pi_1} j_{\pi_2} \ldots j_{\pi_k}\rangle \langle i j_1 j_2 \ldots j_k|, \tag{4}$$

where the sum is done over $i \in \{1, \ldots, d_A\}$ *and* $j_1, \ldots, j_k \in \{1, \ldots, d_B\}$*.*

Then τ is symmetric under all permutations of $\mathcal{H}_{\mathrm{B}_1} \otimes \ldots \otimes \mathcal{H}_{\mathrm{B}_k}$ if $P_\pi \tau = \tau P_\pi$ for all $\pi \in \mathcal{S}_k$.

The second variant uses the following.

Definition 4. *The symmetric subspace of* $\mathcal{H}_{B_1} \otimes \ldots \otimes \mathcal{H}_{B_k}$ *has a basis composed of elements of the form:*

$$\frac{1}{\mathrm{cte}} \sum_{\pi \in \mathcal{S}_k} |j_{\pi_1} j_{\pi_2} \ldots j_{\pi_k}\rangle, \qquad 1 \leqslant j_1 \leqslant j_2 \leqslant \ldots \leqslant j_k \leqslant d_B. \tag{5}$$

We write these elements $|\omega_\ell\rangle$*, with the index* $\ell = 1, \ldots, L$ *running over all* $j_1 \ldots j_k$ *satisfying the order condition above. For each* $|\omega_\ell\rangle$*, the constant is chosen such that the resulting coefficients are 0/1.*

Proposition 5. *An operator* $\tau \in \mathsf{Lin}(\mathcal{H}_A \otimes \mathcal{H}_{B_1} \otimes \ldots \otimes \mathcal{H}_{B_k})$ *obeys the "support and range" condition of Definition 2 if* τ *can be written:*

$$\tau = \sum_{i_1 i_2 \ell_1 \ell_2} \beta_{i_1 i_2 \ell_1 \ell_2} |i_1\rangle \langle i_2| \otimes |\omega_{\ell_1}\rangle \langle \omega_{\ell_2}| \tag{6}$$

for complex coefficients $\beta_{i_1 i_2 \ell_1 \ell_2}$*.*

1.2 PPT constraints

For $1\leqslant c\leqslant k$, we define the partial transpose operation $\top_c$ such that $\top_c[\tau]=\tau^{\top_{\mathrm{B}_1}\cdots\top_{\mathrm{B}_c}}$. Precisely, if

$$\tau=\sum_{ii'j_1j_1'\ldots j_kj_k'}\beta_{ii'j_1j_1'\ldots j_kj_k'}|i\,j_1\ldots j_k\rangle\langle i'\,j_1'\ldots j_k'|, \tag{7}$$

then

$$\top_c[\tau]=\sum_{ii'j_1j_1'\ldots j_kj_k'}\beta_{ii'j_1j_1'\ldots j_kj_k'}|i\,j_1'\ldots j_c'j_{c+1}\ldots j_k\rangle\langle i'\,j_1\ldots j_cj_{c+1}'\ldots j_k'|. \tag{8}$$

The positive partial transpose constraints are given by $\top_c[\tau]\succcurlyeq 0$ for each $c\in C$.

2 Semidefinite formulation using equality constraints

This form is called the primal form in the documentation of most primal-dual solvers such as SeDuMi [?], SDPT3 [?], etc...

It is *not* the default form provided by YALMIP, however, the setting `dualize` can be set to 1 to employ this form. It *seems* to be the form preferred by CVX version 2 (**verify**); however, CVX version 3 can formulate problems in either the primal or the dual form; this is controlled by the command `cvx_dualize`.

2.1 Without using the "support and range" condition

Primal variables. — Our variables are $\sigma\in\mathsf{Herm}_+(\mathcal{H}_\mathrm{A}\otimes\mathcal{H}_\mathrm{B})$, the element of our approximation $\tilde{\mathsf{S}}$, and the extension $\tau\in\mathsf{Herm}_+(\mathcal{H}_\mathrm{A}\otimes\mathcal{H}_{\mathrm{B}_1}\otimes\ldots\otimes\mathcal{H}_{\mathrm{B}_k})$.

Equality constraints. — The extension reproduces the bipartite state:

$$\mathrm{tr}_{\mathrm{B}_2\ldots\mathrm{B}_k}[\tau]=\sigma, \tag{9}$$

and the extension is symmetric:

$$\Pi\tau\Pi=\tau, \tag{10}$$

where $\Pi=\sum_\pi P_\pi$ is the projection onto the symmetric subspace.

Remarks. — The semidefinite constraints $\tau\succcurlyeq 0$ and $\sigma\succcurlyeq 0$ are automatically present in the primal form and do not need to be added manually.

When the symmetric extension is contained in a larger semidefinite program, the variable σ can well be represented by linear combinations of other variables. In that case, it is not necessary to define an additional semidefinite variable σ; instead, the equality constraints can be modified accordingly.

2.1.1 PPT constraints

Additional primal variables. — Each PPT constraint $c\in C$ requires a new variable $\rho_c\in\mathsf{Herm}_+(\mathcal{H}_\mathrm{A}\otimes\mathcal{H}_{\mathrm{B}_1}\otimes\ldots\otimes\mathcal{H}_{\mathrm{B}_k})$.

Additional equality constraints. — We require:

$$\rho_c=\top_c[\tau]. \tag{11}$$

2.1.2 Final remarks

While conceptually simple, this formulation is not particularly efficient due to the high number of equality constraints in (10) and the large dimension of the matrices. The next section provides a more efficient formulation.

2.2 With the "support and range" condition

We use the following parameterization of τ, when its support and range is restricted to the symmetric subspace.

Proposition 6. *Let L be the size of the symmetric subspace in Definition 4, and we write $\mathcal{H}_L = \mathbb{C}^L$. Then τ obeys the "support and range" condition if there exists $\hat{\tau} \in \mathsf{Herm}(\mathcal{H}_A \otimes \mathcal{H}_L)$ such that*

$$\tau = (\mathbb{1}_A \otimes \Omega)\, \hat{\tau}\, (\mathbb{1}_A \otimes \Omega)^*, \tag{12}$$

where Ω represents the change of basis from $\mathcal{H}_L$ to $\mathcal{H}_{B_1} \otimes \ldots \otimes \mathcal{H}_{B_k}$:

$$\Omega = \sum_{\ell} |\omega_\ell\rangle\langle \ell| \in \mathbb{C}^{L \times d_{\mathrm{B}}^k}. \tag{13}$$

Note: Ω is obtained by simply concatening the column vectors corresponding to $|\omega_\ell\rangle$.

Primal variables. — Our primal variables are $\sigma \in \mathsf{Herm}_+(\mathcal{H}_{\mathrm{A}} \otimes \mathcal{H}_{\mathrm{B}})$, the element of our approximation $\tilde{\mathsf{S}}$, and the parameterization $\hat{\tau} \in \mathsf{Herm}_+(\mathcal{H}_{\mathrm{A}} \otimes \mathcal{H}_{\mathrm{L}})$. Positive semidefinitiveness of both is implied by the primal formulation. Note that $\hat{\tau} \succcurlyeq 0$ implies $\tau \succcurlyeq 0$.

Equality constraints. — We have a single equality constraint, that the extension reproduces the bipartite state:

$$\mathrm{tr}_{\mathrm{B}_2 \ldots \mathrm{B}_k}[(\mathbb{1}_{\mathrm{A}} \otimes \Omega)\, \hat{\tau}\, (\mathbb{1}_{\mathrm{A}} \otimes \Omega)] = \sigma. \tag{14}$$

2.2.1 PPT constraints

Each PPT constraint $c \in C$ breaks the symmetry of $\mathcal{H}_{\mathrm{B}_1} \otimes \ldots \otimes \mathcal{H}_{\mathrm{B}_k}$; instead, ρ_c has support and range in the symmetric subspaces of $\mathcal{H}_{\mathrm{B}_1} \otimes \ldots \otimes \mathcal{H}_{\mathrm{B}_c}$ and $\mathcal{H}_{\mathrm{B}_{c+1}} \otimes \ldots \otimes \mathcal{H}_{\mathrm{B}_k}$. We reuse the trick of Proposition 6 by introducing the bases $\{|\omega'_\ell\rangle\}$ and $\{|\omega''_\ell\rangle\}$ of these respective symmetric subspaces, with respective dimension L' and L''.

Additional primal variables. — The additional variable $\hat{\rho}_c \in \mathsf{Herm}_+(\mathcal{H}_{\mathrm{A}} \otimes \mathcal{H}_{\mathrm{L}'} \otimes \mathcal{H}_{\mathrm{L}''})$ parameterizes

$$\rho_c = (\mathbb{1}_{\mathrm{A}} \otimes \Omega' \otimes \Omega'')\, \hat{\rho}_c\, (\mathbb{1}_{\mathrm{A}} \otimes \Omega' \otimes \Omega'')^*, \tag{15}$$

where Ω' represents the change of basis from $\mathcal{H}_{\mathrm{L}'}$ to $\mathcal{H}_{\mathrm{B}_1} \otimes \ldots \otimes \mathcal{H}_{\mathrm{B}_c}$:

$$\Omega' = \sum_{\ell'} |\omega'_{\ell'}\rangle\langle \ell'| \in \mathbb{C}^{L' \times d_{\mathrm{B}}^c}, \tag{16}$$

and Ω'' represents the change of basis from $\mathcal{H}_{\mathrm{L}''}$ to $\mathcal{H}_{\mathrm{B}_{c+1}} \otimes \ldots \otimes \mathcal{H}_{\mathrm{B}_k}$:

$$\Omega'' = \sum_{\ell''} |\omega''_{\ell''}\rangle\langle \ell''| \in \mathbb{C}^{L'' \times d_{\mathrm{B}}^{k-c}}. \tag{17}$$

Additional equality constraints. — We require:

$$\rho_c = \top_c[(\mathbb{1}_{\rm A}\otimes\Omega'\otimes\Omega'')\,\hat{\rho}_c\,(\mathbb{1}_{\rm A}\otimes\Omega'\otimes\Omega'')^*]. \tag{18}$$

Note: implemented naively, this adds many redudant equality constraints, causing numerical instability. Instead, write, for $i_1, i_2 = 1, ..., d_{\rm A}$ and $\ell_1', \ell_2' = 1, ..., L'$ and $\ell_1'', \ell_2'' = 1, ..., L''$:

$$\langle i_1 \ell_2' \ell_1'' | \hat{\rho}_c | i_2 \ell_1' \ell_2'' \rangle = \langle i_1 \ell_1 | \hat{\tau} | i_2 \ell_2 \rangle. \tag{19}$$

We left undefined the relations $\ell_1 = f(\ell_2', \ell_1'')$ and $\ell_2 = f(\ell_1', \ell_2'')$.

The function f is defined as $\ell \equiv f(\ell', \ell'')$, with $1 \leqslant \ell \leqslant L$, $1 \leqslant \ell' \leqslant L'$, $1 \leqslant \ell'' \leqslant L''$. To obtain ℓ, we first decompose take a nonzero $|j_1 ... j_c\rangle$ present in $|\omega_{\ell'}'\rangle$, and a nonzero $|j_{c+1} ... j_k\rangle$ present in $|\omega_{\ell''}''\rangle$. The basis $|\omega_\ell\rangle$ containing a nonzero $|j_1 ... j_k\rangle$ gives the required ℓ.

3 Semidefinite formulation using inequality constraints

Let $\{\alpha_i\} \in \mathsf{Herm}(\mathcal{H}_{\rm A})$ and $\{\beta_j\} \in \mathsf{Herm}(\mathcal{H}_{\rm B})$ be bases of their respective spaces, such that $\alpha_1 = \mathbb{1}_{\rm A}$ and $\beta_1 = \mathbb{1}_{\rm B}$, and $i = 1, ..., d_{\rm A}^2$ while $j = 1, ..., d_{\rm B}^2$. These bases should be orthogonal, but not necessarily normalized.

Then, the operator $\sigma \in \mathsf{Herm}(\mathcal{H}_{\rm A} \otimes \mathcal{H}_{\rm B})$ has a decomposition:

$$\sigma = \sum_{ij} s_{ij} (\alpha_i \otimes \beta_j), \tag{20}$$

while its symmetric extension τ has the decomposition:

$$\tau = \sum_{i j_1 ... j_k} t_{i j_1 ... j_k} (\alpha_i \otimes \beta_{j_1} \otimes ... \otimes \beta_{j_k}), \tag{21}$$

with the constraint that $t_{ij1...1} = s_{ij}$ and that $t_{i j_{\pi_1} ... j_{\pi_k}} = t_{i j_1 ... j_k}$ for all permutations $\pi \in \mathcal{S}_k$.

Dual variables. — The coefficients $t_{i j_1 ... j_k}$ are variables of our formulation, with the following exceptions:

- when the $j_1 ... j_k$ are not sorted in increasing order, the coefficient $t_{i j_1 ... j_k}$ is an alias for $t_{i j_1' ... j_k'}$ where $(j_1', ..., j_k')$ are the indices $(j_1, ..., j_k)$ sorted in increasing order (note: "increasing" is actually "nondecreasing", due to possible repetitions in the index values),
- the coefficient $t_{i j_1 1 ... 1}$ is directly set to the value $s_{i j_1}$.

These coefficients are all real but otherwise unrestricted. If the symmetric extension is part of a larger semidefinite program, the coefficients s_{ij} can be replaced by the relevant (linear) expressions.

Then the constraint:

$$\tau = \sum_{i j_1 ... j_k} t_{i j_1 ... j_k} (\alpha_i \otimes \beta_{j_1} \otimes ... \otimes \beta_{j_k}) \geqslant 0 \tag{22}$$

correspond to the canonical form of the solver.

PPT constraints. — These constraints are easy to incorporate. For $c \in C$, simply add:

$$\sum_{i j_1 ... j_k} t_{i j_1 ... j_k} (\alpha_i \otimes \beta_{j_1}^\top \otimes ... \otimes \beta_{j_c}^\top \otimes \beta_{j_{c+1}} \otimes ... \otimes \beta_{j_k}) \geqslant 0. \tag{23}$$

3.1 Restriction to the symmetric subspace

By an appropriate restriction to the symmetric subspace, the formulation above can be improved. The constraint (22) can be imposed only on the subspace defined by $|ij_1...j_k\rangle$ when the $j_1...j_k$ are in increasing order. Note that in the present subsection, i and $j_1...j_k$ are indices of the bra-ket computational basis, not the indices of the Hermitian basis.

This corresponds to dropping rows and columns of the matrices in the dual constraint (22). For the PPT constraints, the story is similar, except that we require only that the indices $j_1...j_c$ on the one hand, $j_{c+1}...j_k$ on the other hand to be increasing.

However, this formulation introduce linear dependences in blocks of the problem, and can lead to numerical instabilities.